

RA
11
B1873
no. 1703
1967

Berman, Mones
USERS MANUAL FOR SAAM
(Stimulation, Analysis and Modeling)

D 50280
>>#0.54

RA11
.B1873
no.1703
1967

845

4781

SAAM manual

LIBRARY
JAN 2 1968
NATIONAL INSTITUTES OF HEALTH

U.S. DEPARTMENT OF
HEALTH, EDUCATION, AND WELFARE
PUBLIC HEALTH SERVICE

USERS MANUAL FOR

S A A M

(Simulation, Analysis and Modeling)

by

Mones Berman and Marjory F. Weiss

National Institute of Arthritis and Metabolic Diseases,

National Institutes of Health, Bethesda, Maryland

For sale by the Superintendent of Documents, U.S. Government Printing Office
Washington, D.C. 20402 - Price \$1.25

PHS publication no. 1703

RAII
B1873
no. 1703
1967

TABLE OF CONTENTS

Sections

	Foreword
I	Introduction
II	General Features
III	Input
IV	Output
V	Diagnostics
VI	Model Types
VII	Computational Procedures and Methods
VIII	Program Organization
IX	Comments and Suggestions
X	Sample Problems
XI	References
XII	Appendix

FOREWORD

SAAM is a digital computer program developed for the analysis of data in terms of models. It permits simulation and data fitting, and contains various techniques encountered in model building.

Although developed primarily for biological systems and more specifically for kinetic models, the program is of general utility. It differs from other simulation and analysis systems in that the "language" is geared towards the bio-medical "system" investigator and its elements are direct counterparts of techniques and conceptualizations used by the experimenter.

Model building is complicated and requires--in addition to intuition and speculation--knowledge of mathematical and statistical procedures and their limitations. This manual is only a brief description of the procedures used in SAAM and some of their limitations. For additional background material the reader is referred to the reference section.

SAAM is a large, complex program and is continuously being extended and revised. Like any large program, SAAM is difficult to completely debug, and it probably contains some undetected errors, even though it has been in use since 1959. It is recommended, therefore, that the user run some test problems of his own, the answers to which he knows. We also invite users to call to our attention any questionable results which may be attributed to the program and not to errors in the data.

This manual is for the SAAM 23 version of the program. Revisions and updates will appear occasionally, and will be sent to those who request that their names be placed on our mailing list. A new version of SAAM is

now under development and will be known as SAAM 24. SAAM 24 will contain major revisions and many new features, and a completely new manual will be written for it.

SECTION I

INTRODUCTION

INTRODUCTION

SAAM is a general purpose computer program designed to fit physical or mathematical models to data by adjusting the parameter values of the model until a "best" fit is obtained. Any set of mathematical equations (differential, integral or algebraic) or functions may serve as a model provided an analytical or numerical procedure exists for its solution. An open-ended library of model types is incorporated within the program for routine use. A partial list of the model types included in the SAAM library is given in Section II.

The program uses a common data input format for all types of models. This is made possible through the use of a single set of operational elements in the program and a defined equivalence between these elements and the elements of each model type. SAAM permits the acceptance of "raw" experimental data. The number of entries required for the specification of models and constraints has been minimized to simplify use.

As will be discussed more fully later, SAAM contains a number of features designed to aid an investigator in his model building efforts. As a result, the program has become quite large.

The SAAM 22 version of the program is in FORTRAN II (with a few subroutines in FAP), contains over 200 subroutines and about 15,000 FORTRAN statements. It is compiled under the IBM independent FORTRAN monitor for routine execution in an IBM 7094 using the CHAIN facility. A CHAIN tape generated from the relocatable binary links is saved for routine use. At execution time the preaddressed CHAIN tape is mounted and a short MAIN program is loaded to call in the first link. Subsequently, particular

links are brought into core as each problem requires.

The SAAM 22 version has also been converted to FORTRAN IV and compiled for routine use on the CDC 3600 and CDC 6600 systems.

The SAAM 23 version is a revised version of SAAM written in FORTRAN IV. Most of the modifications are minor and need not concern the user. Problem decks run with SAAM 22 will also run with SAAM 23.

Problems to be run are loaded behind the MAIN program. Further details on the organization of SAAM into blocks are presented in Section VIII of this manual.

SECTION II

GENERAL FEATURES

COMPUTATIONAL STRUCTURE

Formally we can describe a system or a model by its responses, a set f_i :

$$f_i = F_i(\lambda, f_o, t)$$

where F_i is the functional relation of f_i to a set of parameters .

$\lambda(\lambda_1, \lambda_2, \dots, \text{etc.})$, some set of condition values $f_o(f_{o1}, f_{o2}, \dots)$

that characterize constraints (such as initial or boundary conditions),

and some independent variables $t(t_1, t_2, \dots)$.

Experimental data (q_j^o) are observables of the system and as such are estimates of some theoretical values q_j that are functions of the f_i :

$$q_j = G_j(f_i).$$

In these terms, the fitting of a model to data implies the derivation of a set of parameter values for which the q_j will "best" fit the data, q_j^o .

This involves three stages of computations:

- 1) equations solution - to calculate f_i given a set of values for the λ and f_o .
- 2) matching - to convert the f_i to the theoretical q_i .
- 3) parametric fitting - to adjust the λ values until the q_i "best" fit the data q_i^o .

When the functional relation F_i and/or the number of parameters, λ , are unknown, the fitting of a model to data also implies derivation of an F_i and a set of λ 's. This is referred to as model building, and will be considered only briefly in this manual.

1. Solution of equations

This stage calculates f_i , given a set of λ and f_o . The

computations depend on the type of model and on the available computational methods. For example, differential equations are solved

numerically using a 4th order Runge-Kutta method (7). Linear differential equations with constant coefficients can also be solved using an eigenvalue-eigenvector method or--in special cases--using an analytic method. Each method of solution is executed by a separate subroutine. Each subroutine calculates values for f_i required for the calculations of any q_i requested in a problem. The q_i requested may correspond to observations q_i^0 or to any simulated quantity of interest.

The subroutines for the solution of different model types are stored in a library of "models". During the execution of a particular problem the appropriate subroutines are brought into core memory.

2. Matching

An observation, q_j^0 , is a measure of some function, q_j , of the set of solution values f_i that characterize the system or model. Due to experimental constraints the q_j need not correspond directly to the f_i . Although various functional relations between the q_j and f_i are possible, at present only linear relations are provided for:

$$q_j = \kappa_j \sum_i \sigma_{ji} f_i$$

The f_i required for the calculation of the q_j are computed and stored in the equations solution stage. If the σ_{ji} are known from the experimental set up, the q_j can be calculated directly. If the σ_{ji} are not known, their values may be estimated from the observed quantities q_j^0 :

$$q_j^o = \kappa_j \sum_i \sigma_{ji} f_i$$

using a least squares linear regression analysis (8), provided the number of independent observations is equal to or greater than the number of unknown σ_{ji} . With the σ_{ji} thus determined, the q_j can be calculated.

In the structure of SAAM the σ_{ji} appear as secondary parameters, as distinguished from the λ_{ji} which are primary parameters.

The calculation of a specified set of q_j , given a model and values for λ , f_o , and σ , is referred to as simulation and is equivalent to the same process performed on an analog computer.

3. Parametric fitting of data

This stage involves the adjustment of the model parameters, λ , until the calculated q_j "best" approximate the observations q_j^o . In general, the q_j are non-linear functions of the λ , and a non-linear least squares fitting procedure is employed. Starting with initial estimates for the parameter values, one calculates a set of q_j . Adjustment of the initial λ values is then made using a first order approximation.

$$\delta q_j = \sum_i \frac{\partial q_j}{\partial \lambda_i} \delta \lambda_i$$

The partial derivative of each q_j with respect to λ is obtained as an approximation by calculating a Δq_j for a small change $\Delta \lambda_i$ and setting

$$\frac{\partial q_j}{\partial \lambda_i} = \frac{\Delta q_j}{\Delta \lambda_i}$$

The δq_j are approximated by the difference between the observed and

calculated q_j

$$\delta q_j = q_j^o - q_j$$

so that





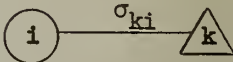
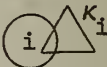
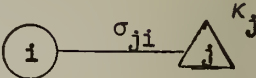

$$\sum \frac{\Delta q_j}{\Delta \lambda_i} \delta \lambda_i = q_j^o - q_j$$

This constitutes a set of equations from which, using linear regression analysis, a set of $\delta \lambda_i$ can be calculated to minimize $(q_j^o - q_j)^2$. Since q_j are non-linearly related to the λ_i , the above procedure is only an approximation to a least squares fit and is iterated until convergence is achieved.

In the neighborhood of a least squares fit this procedure yields a variance-covariance matrix for the λ . From this matrix are calculated estimates for the standard errors of the λ and their correlation coefficients. These estimates, however, do not necessarily reflect the true uncertainties in the λ 's due to non-linearities in the q_j with respect to the λ_i .

MODEL TYPES IN PROGRAM LIBRARY

Different types of models can be processed by the program. Each type of model is coded so that the data deck will be correctly interpreted. To simplify the preparation of data a common nomenclature and data form have been adopted for all types of models, and equivalences are defined between the parameters of the model type and the common nomenclature. Operational units and graphical symbols are introduced as aids in describing the equivalences. A detailed discussion of each model type is given in Section VI on Model Types.

Program Element	Description	Symbol
$f_i(t)$	function i	
$f_i(0)$	initial value of $f_i(t)$ at $t = 0$	$f_i(0)* \longrightarrow$ 
$q_k(t)$	composite function k , a function of one or more f_i 's	
λ_{ji}	primary parameter	
σ_{ki}	secondary parameter: summing coefficient $q_j = \sum_{i \neq k} \sigma_{ki} f_i$	
κ_i	secondary parameter: proportionality coefficient $q_i = \kappa_i f_i$	
or		
	$q_j = \kappa_i \sum_{i \neq j} \sigma_{ji} f_i$	
F_j	function generator j	
t	independent variable	
θ	second independent variable	
M_i	matrix i	

SECTION III

INPUT

INPUT FORMAT

A number of headings are used in setting up a problem. These are described in this section in the order required by the program. The formatting of information under each heading makes use of two types of fields: integer, and decimal.

Integer fields require that no decimal point be entered, and that the number be at the right end of the field.

Decimal fields permit the number to be entered anywhere in the indicated field but the decimal point must be entered, even for a whole number.

The problem deck is organized in sections which must be in the following order:

A. Required sections:

1. card 1 - clock option and problem I.D.
card 2 - number of components and number of iterations
card 3 - timing and convergence criteria
card 4 - options and model type
2. data
'26'(termination card*)
3. initial conditions
'26'
4. Kappas
'26'
5. Lambdas
'26'
6. Sigmas
'26'
7. Dependence Relations
'26'
8. Statistical constraints
'26'

B. Additional sections as required by the problem:

1. T-interrupt changes in f_i
'26'
'26'
2. T-interrupt changes in parameters.
'26'
3. Normal equations entries

C. Special entries

These are required only for particular model types. How and where they are to be entered are described under model type.

*Footnote - for required sections (2 through 8) the termination cards '26' must be present whether or not other cards are entered.

LIMITS IMPOSED BY PROGRAM

Because of physical limitations in the computer the following limits are, at present, imposed by the SAAM program:

Number of components	≤	25
Number of primary and secondary parameters	≤	60
Number of dependence relations	≤	34
Number of variable parameters	≤	25
Number of data and "statistical constraints"	≤	250
Number of T-interrupts	≤	4

CARD 1

	PROGRAM I.D.	PROBLEM I.D.		USERS NAME AND DESCRIPTION OF PROBLEM	
		INIT.	NUMBER		
1	3 → 8	10 → 12	13 → 20	22 →	72
	SAAM 23				73 → 80

CARD 1

Column 1. Enter a "1" or "2" to clue the program that this is the beginning of a problem deck.

The "2" is used when an ON-LINE clock is available on the computer. This will result in a printout of the starting time for a problem and its elapsed execution time. A "1" in this field will bypass the clock.

Column 3 → 8. Enter "SAAM 23" to identify the version of the program used.

Column 10 → 21. Problem identification number: three initials followed by up to nine characters (numbers, letters, decimals).

Column 23 → 72. Users name and description of problem.

User is free to enter whatever he wishes in this field. It will be printed in the output as is.

Card 2

		No. of Components (integer)	No. of Iterations (integer)										
1	2+5	6+10	19	20	29	30	49	50	51 + 55	56 + 60	61 + 65	66 + 70	73 + 80

CARD 2

Column 19 → 20. Number of components. This corresponds to the largest index associated with any component of the model.

Column 29 → 30. Maximum number of iterations for least squares convergence. Computation may be terminated internally before this maximum is reached if convergence criteria are satisfied.

"Blank" or "zero" entry in this field is interpreted as ZERO ITERATIONS and results in just one solution based on initial values of primary parameters. With secondary parameters fixed this^{is} equivalent to a SIMULATION.

	TIME FACTOR (decimal)		P (decimal)	P ₁ (decimal)	E (decimal)		CONMIN (decimal)	
1	2 → 10	11 → 20 ,	21 → 30	31 → 40	41 → 50	51 → 60	61 → 70	73 → 80
				.01	.98		.98	

CARD 3

Column 2 → 10. "Blank" unless the internally allotted time for a single solution of the differential equations is to be modified.

Internally allotted time is 0.5 units. (Computational units)

Enter smaller or larger value as desired.

Column 21 → 30. "Blank". See Section VII-5 for additional information.

Column 31 → 40. Enter ".01". This entry indicates fractional change

in parameter λ used to calculate $\partial q / \partial \lambda$. Usual entry .01.

Column 41 → 51. This is convergence test value. Usual entry .98.

Column 61 → 70. This is also convergence test value. Usual entry .98.

CARD 4

- Column 2. "Blank" - no print or punch of covariance matrix.
"1" - print and punch covariance matrix.
- Column 3. "Blank" - no printout of partials matrix.
"1" - printout of partials matrix.
- Column 4. Plotting options:
"Blank" - no plots
"1" - semi-log 2 page plot.
"2" - semi-log 1 page plot.
"3" - linear 2 page plot.
"4" - linear 1 page plot.
- Column 5. "Blank" - no print or punch of A matrix.
"1" - print and punch A matrix.
- Column 6. "Blank" - no print of intermediate results.
"1" - print intermediate results.
- Column 49 → 50. Type of model solution.
"Blank" - program will choose automatically
among solutions 1, 2 and 4.
integer entry - number corresponding to desired
model type. (See code in section on model types .)

DATA

This heading permits the specification of functions to be calculated for simulation or for the fitting of data. The function numbers (i), the independent variables (t, θ), observed values (q_i^0) and the statistical weights are entered as follows:

column 2 \rightarrow 5. Component number - specifies subscript i of

$q_i(t, \theta)$ (function or summer) as defined by the model code.

column 13 \rightarrow 25. Value of independent variable t .

column 27 \rightarrow 40. Observed value $q_i^0(t, \theta)$, if available.

column 42 \rightarrow 55. Relative statistical weight of observed value.

column 57 Blank

column 59 \rightarrow 72. Independent variable θ .

Each line under this format constitutes a request for a single computation $q_1(t, \theta)$. The execution sequence of computational requests may be changed internally by the program.

Control Cards

- 1) Entry control card (EC): modifies, defines or interprets the entries on the data cards that follow it. Control is terminated by a new entry control card or by the termination of entries under the DATA heading. A control card is not considered a datum.

column 2 → 5. Entry of 100. + X. Designates an EC card and assigns X to all succeeding entries under COMP, except when X = 0. When X = 0. COMP entries remain unchanged. For example, an entry 103. will assign a COMP No. 3. to all succeeding entries; a 100. will leave them unchanged.

column 13 → 25. An entry X in this field will add X to all entries that follow in this field. This provides for a shift in the "t" coordinate. X may be positive or negative.

column 27 → 40. An entry X in this field multiplies by X all entries that follow in this field. When X = 0, or blank, the entries that follow remain unchanged.

column 42 → 55 and column 57 are used jointly as a code for statistical weight assignment as follows:

Entry Control Card		Interpretation of weight field (columns 42 + 55) of succeeding cards
Columns 42 + 55	column 57	
blank	blank	relative weight
blank	1	standard deviation of observations
x	1	standard deviation of observed value equals X. data card weight field ignored
x	2	coefficient of variance of observed value equals X. data card weight field ignored X must be non zero

Note: 1) Weights are calculated and normalized by the program when the standard deviations or coefficient of variance are given.

2) SAAM assigns zero weight whenever the given or calculated standard deviation is zero.

3) The weight assignments for a given problem must be compatible.

Either relative weights or weights based on standard deviations must be used exclusively. Both types of weighting will not be accepted in a single problem.

4) See section on Methods for discussion of statistical weights and the calculation of SIG.

2) t-interrupt control card (TC): interrupts the computations and permits changes to be introduced during the solution of a problem. Specifically, at any specified "t", existing parameter values may be switched to new values, and Δf_i may replace or be added to the values f_i existing at "t".

column 2 → 5. The entry "126." signifies a TC card effective at the t-value assigned to the datum immediately preceding it. This remain in effect until another TC card or termination card is encountered. (EC cards work independently of the TC cards.)

column 12 → 25.

- a) A blank in this field indicates that the t-values of the data that follow are to be interpreted with respect to a new t scale starting with $t = 0$ at the TC card.
- b) A "1." in this field indicates that the t-values of the data that follow refer to the same t scale as those preceding the TC card.

column 27 → 40.

- a) A blank in this field indicates that a new set of f_k values replace the current f_k values at the t-interrupt. The new values are specified under "t-interrupt changes in f_1 ."
- b) A "1." in this field indicates that a set of values Δf_k (entered under "t-interrupt changes in f_k ") are to be added to the existing f_k at the t-interrupt.

column 42 → 55. Blank.

column 57. Blank

column 59 → 72. Blank

- 3) Data Generation Control Card. (GC): is used as an expedient to generate "artificial" data. This control card generates X

May 1966

data entries at intervals Δt starting with the t-value of the last datum (entered or generated). The component number and weight of the last datum (entered or generated) is carried over to the generated entries. A number of GC cards can follow each other.

column 2 \rightarrow 5. The entry "200." signifies a GC card

column 12 \rightarrow 25. Enter Δt , the t-interval between generated data points.

column 27 \rightarrow 40. Blank

column 42 \rightarrow 55. Enter X, the number of data points to be generated.

column 57. Blank

column 59 \rightarrow 72. Blank

This heading permits the entry of $f_i(0)$ values for each component i .

Only non-zero entries need be made.

column 4 → 5 component number, i

column 12 → 25 initial conditions $f_i(0)$

column 42 → 55 V

column 56 → 70 U

PARAMETERS

SAAM recognizes three types of parameters: KAPPAS, LAMBDA and SIGMAS. The LAMBDA are usually non-linearly related to the functions $f_i(t)$ and require iterative adjustment for a least squares fit. The SIGMAS and KAPPAS are linear functions of the observations. The hierarchy of computations in the program is as follows:

$$f_i = F_i(\lambda, f_0, t, \theta)$$

$$q_i = \kappa_i f_i \quad \text{or} \quad q_j = \kappa_j \sum_{i \neq j} \sigma_{ji} f_i$$

All parameters are doubly subscripted, although the second subscript of Kappas (always zero) is frequently omitted.

From the point of view of adjustment of parameters to fit data, the parameters are classified as:

fixed: the parameter takes on preset values
assigned in advance.

dependent: parameter takes on a value as prescribed by a
dependence relation.

adjustable: parameter is free to adjust as required by the
program in data fitting.

Fixed parameters may change during a solution but always in a pre-determined manner, independent of the fit. Such changes may occur, for example, in connection with a t-interrupt.

Dependent parameters are usually dependent on other parameters and/or constants and

are indirectly adjusted in connection with the fitting of data.

A parameter, once classified as dependent, remains so throughout the

solution and always obeys the same functional dependence relation.

A parameter is designated as dependent by a code on its entry card ("1" in column 60). The dependence relation is specified under a separate entry (Dependence relations).

At present dependence relations are restricted to linear relations only, such as

$$P_{ij} = \sum_{k,h} a_{kh} P_{kh}$$

The parameter P_{ij} on the left side is the dependent one and the P_{kh} on the right side of the equation can be fixed, dependent or adjustable. The program resolves these dependence relations internally, so that dependent parameters are finally expressed in terms of adjustable and fixed parameters only.

Whereas sigmas and kappas can be dependent on other sigmas, kappas, lambdas, or constants, lambdas can be dependent only on lambdas and constants.

Adjustable parameters have upper and lower limits assigned to them. These limits are never violated in adjusting the parameter during data fitting. The program identifies a parameter as adjustable because its upper limit is greater than its lower one.

An adjustable parameter is entered with an initial estimate* and a maximum and minimum limit. In addition, an estimate of a standard deviation can also be entered, when known a priori. Such information may be known from sources other than the data to be fitted. The standard

*Initial estimates are not required for sigmas and kappas unless a standard deviation is given for them.

deviation is associated with the initial estimate value and is combined statistically with the data by the program to derive best estimates for the adjustable parameters. More extensive statistical constraints can also be entered under the separate heading "STATISTICAL CONSTRAINTS".

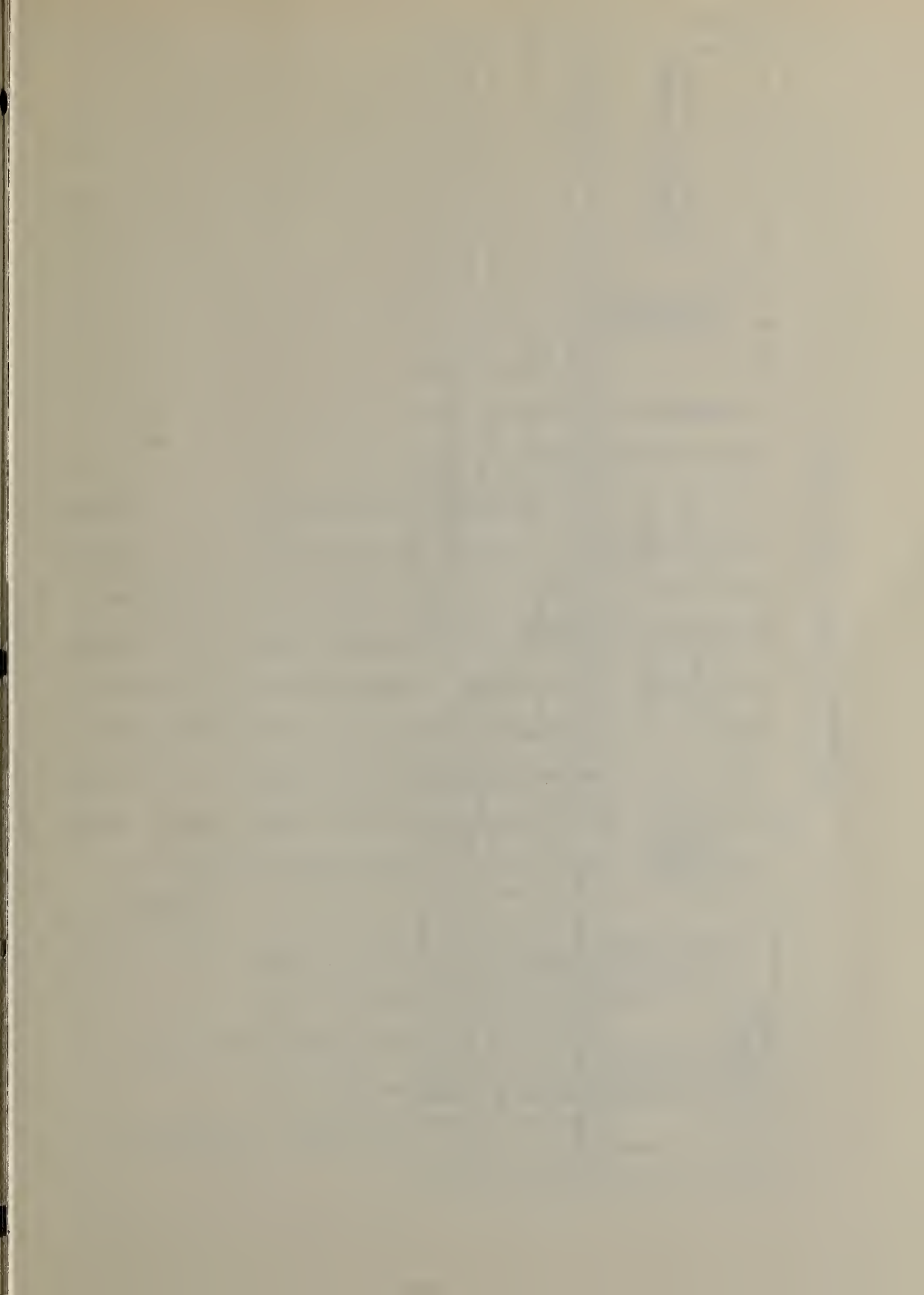
It may be noted that the statistical constraints on a parameter are independent of the upper and lower limits. The latter are not involved in calculating corrections for the adjustable parameters but are used to limit the corrections to within the specified region.

Parameters can also be f-dependent. This means that during computations their values are modified by an $f_i(t)$ for every t . f -dependence is restricted to two forms: the parameter value is multiplied or divided by some $f_i(t)$. At present only model type 4 permits f -dependence.

The kappas are read first by the program. Before reading this category the program automatically assigns fixed values $\kappa_i = 1$. for all components of the model. These values are overwritten by the κ_i entries. Therefore only $\kappa_i \neq 1$ need be entered.

The lambdas are entered next followed by the sigmas. Only lambdas and sigmas required in the model need be entered.

The order of the entries under each heading is not critical.



column 4 → 5. 1st subscript of parameter.

column 9 → 10. 2nd subscript of parameter. For KAPPAS second subscript is always zero.

column 12 → 25. Value of parameter. This field is ignored by the program for variable SIGMAS and KAPPAS unless STANDARD DEVIATION field (62 → 72) has a non-zero entry.

column 27 → 40. Lower limit for adjustable parameter.

column 42 - 55. Upper limit for adjustable parameter. Upper limit must always be greater than lower limit for all adjustable parameters.

column 57 → 59. Blank: if there is no f-dependence.

+ i: if parameter is to be multiplied by $f_i(t)$ throughout the computation.

- i: if parameter is to be divided by $f_i(t)$ throughout the computation.

column 60 : Blank: if parameter is fixed or adjustable.

"1": if parameter is dependent. Dependence

relations are entered separately under "DEPENDENCE RELATIONS"

column 62 → 72: enter X for adjustable parameter only when the

value, P, of the parameter is known with a standard deviation

± X : value = P ± X.

SUMMARY OF INFORMATION TO BE ENTERED ON A CARD DEFINING A PARAMETER

Type of Parameter	First Subscript	Second Subscript	Value or Initial Estimate	Minimum Limit for Value	Maximum Limit for Value	f-dependence of Parameter	Parameter Dependence	Standard Deviation
	4 → 5	9 → 10	12 → 25	27 → 40	42 → 53	57 → 59	60	62 → 72
Known or fixed λ, σ, κ	X	X	X					
Dependent λ, σ, κ	X	X					1*	
Adjustable λ without Std. Dev.	X	X	X	X	X			
Adjustable σ, κ without Std. Dev.	X	X		X	X			
Adjustable λ, σ, κ with Std. Dev.	X	X	X	X	X			X

Key: X = must be entered

/ = entered if applicable

/// = leave blank

* The '1' entered here is a code notifying SAAM that a dependence relation involving this parameter will be found under the dependence relations heading.

DEPENDENCE RELATIONS

Dependence relations are limited to linear dependences of the type:

$$P_{ij} = \sum_{k,l} A_{kl} P_{kl} + A_{00} \text{ for specified } k \text{ and } l$$

where the P_{kl} are fixed, dependent or adjustable and with the further constraint that λ 's can be dependent only on λ 's.

column 4 → 5. Enter i for dependent λ_{ij} , σ_{ij} or κ_i .

column 9 → 10. a) Enter j for dependent λ_{ij} , σ_{ij} .

b) Leave this field blank for κ_i .

column 19 → 20.

a) Blank for dependence on a constant.

b) Enter i for dependence on λ_{ij} or κ_i .

column 24 → 25

a) Blank for dependence on a constant or κ_i .

b) Enter j for dependence on λ_{ij} or σ_{ij} .

column 27 → 40

- a) Enter the coefficient of the depended-on parameter
- b) Enter a depended-on constant

For example:

$$\sigma_{23} = .5 \lambda_{67} - .7 \sigma_{15} + 16. \kappa_{1,0} + 12.$$

Each term of the dependence relation is entered on a separate card as follows:

4	5	9	10	19	20	24	25	27 → 40		
	2		3		6		7	.5		
	2		3		1		5	-.7		
	2		3		1		0	16.		
	2		3		0		0	12.		

The subscript (0,0) is reserved for a constant.

STATISTICAL CONSTRAINTS

Information is entered under this heading when statistical uncertainty associated with a parameter (λ , σ or κ) or linear combination of parameters is known independently of the data. This is a more general procedure than entering standard deviations directly in columns 62 + 72 of the parameter cards. The latter procedure is used merely for convenience when the statistical constraints apply to a single parameter only and when its estimated value agrees with the initial value employed in the fitting.

If P_{ij} represents parameter i,j , $A_{i,j}$ a constant coefficient, Y an estimated value and X a standard error of the estimate, the general form for statistical constraint may be written as

$$\sum_{i,j} A_{ij} P_{ij} = Y \pm X \quad (\text{for } i,j \text{ involved})$$

This is entered on a number of cards, one for each term. $Y \pm X$ is entered with the last term.

column 4 \rightarrow 5. Enter "i" for λ_{ij} , σ_{ij} or κ_i .

column 9 \rightarrow 10.

a) Enter "j" for λ_{ij} or σ_{ij} .

b) Blank for κ_i .

column 12 \rightarrow 25. The coefficient (A_{ij}) of the parameter entered in

column 4 \rightarrow 10.

column 26 \rightarrow 40. The constant (Y.) on card of last term only.

column 41 \rightarrow 55. The error (X.) on card of last term only.

For example:

$$.7 \lambda_{12} - .5 \sigma_{13,4} + \kappa_1 = 5 \pm 1.$$

4	5	9	10	12 \rightarrow 25	27 \rightarrow 40	42 \rightarrow 55	
	1		2	.7			
1	3		4	-.5			
	1		0	1.	5.	1.	

T-INTERRUPT CHANGES IN f_i

Changes in f_i associated with t-interrupt control cards are entered under this heading. The amounts entered will be added to, or be used in place of, the existing f_i value at the interrupt, as instructed by the TC card (see instructions on TC cards). Two "26" termination for this category are required whenever any t-interrupt (T) cards are involved, regardless of whether or not changes in f_i are to be made.

column 4 → 5. The number, i , of the component whose f_i is to be changed.

column 7 → 20. Amount of change at first t-interrupt (TC1)

column 21 → 35. Amount of change for second t-interrupt (TC2)

column 36 → 50. Amount of change for third t-interrupt (TC3)

column 51 → 65. Amount of change for fourth t-interrupt (TC4)

If no entries are made under this heading for a particular component i , zero entries are automatically assumed internally. This means that "zero" will be either added to or replace f_i , as instructed by the entry on the TC card.

TWO (2) "26" termination cards are required after the last entry under this heading.

T-INTERRUPT CHANGES IN PARAMETERS

The values of fixed and adjustable lambdas, and fixed sigmas and kappas can be changed at each t-interrupt.

To facilitate the description and limitations of this feature, we introduce the following notation:

X_{ij} = value of parameter i,j prior to the start of a solution for $f_i(t)$.

$X_{ij}[TC(K)]$ = value of parameter i,j as set at the K^{th} t-interrupt.

Changes can be made at each t-interrupt in accordance with the following relation:

$$X_{ij}[TC(K)] = A X_{h\ell} + B$$

$X_{i,j}$ and $X_{h,\ell}$ can represent any fixed or adjustable lambdas, or fixed sigmas or kappas and A and B are arbitrary constants.

If any parameter is changed at a t-interrupt, $TC(K)$, all other parameters automatically revert to their values preceding the very first change; $X_{h\ell}$:

$$X_{h\ell}[TC(K)] = X_{h\ell}$$

If no parameter is changed at a TC(K), then all parameters retain their values prior to the TC(K)

$$X_{h\ell}[TC(K)] \equiv X_{h\ell}[TC(K-1)] \text{ for } k > 1$$

$$X_{h\ell}[TC(1)] = X_{h\ell}$$

A "26" card is required as termination of parameter changes for each t-interrupt, regardless of whether or not actual parameter changes are to be made.

column 4 → 5. Enter i for $X_{ij}[TC(K)]$

column 9 → 10. Enter j for $X_{ij}[TC(K)]$

column 12 → 25. Enter constant coefficient A

column 27 → 40. Enter constant B

column 44 → 45. Enter h for $X_{h\ell}$.

column 49 → 50. Enter ℓ for $X_{h\ell}$.

Note: It should be noted that dependent parameters have their values recalculated after each change of parameter values at a t-interrupt.

NORMAL EQUATIONS ENTRY

Frequently it is desired to add to the normal equations generated in the solution of a problem another set of normal equations that represents the aggregate of some previous information. (For example, knowledge of a population of which the single study is a member). Two options are provided. The first option permits the entry of the matrix of normal equations A_p and a vector C_p such that the combined solution will yield

$$(A + \frac{\Sigma}{\Sigma_p} A_p)x = C + \frac{\Sigma}{\Sigma_p} C_p.$$

A and C are the normal equations components normally generated by the model solution. Σ and Σ_p are variances associated with the data and the added normal equations, respectively.

Under option 2, the added normal equations satisfy the combined solution

$$(A + \frac{\Sigma}{\Sigma_p} A_p)x = C + \frac{\Sigma}{\Sigma_p} A_p (\lambda_p - \lambda)$$

where λ_p is a vector of reference values belonging to A_p and C_p , and λ are the values of the adjustable parameters in the problem at the time normal equations are calculated.

Option 1:

- 1) Enter "1" in column 65 of card 4 of the data deck.
- 2) Behind the last card of the deck add the following in the order indicated

- a) a card with the value of Σ_p in columns 21 → 35,

E format

- b) The matrix A_p is entered in accordance with matrix entry format described later. Only one half of the symmetric matrix need be entered.
- c) The vector C_p is entered as a one row matrix, in accordance with matrix entry format.

Option 2:

- 1) Enter "2" in column 65 of card 4 of the data deck.
- 2) Behind the last card of the deck add the following in the order indicated
 - a) a card with Σ_p in columns 21 + 35 (E format).
 - b) The matrix A_p - in accordance with the matrix entry format described later.
 - c) λ_p is entered as a single row matrix.

Note: It is essential, of course, that the order of the adjustable λ 's be the same in the problem and in the added matrix of normal equations.

MATRIX ENTRY FORMAT

The following format is used in the program whenever a matrix is read in for special purposes:

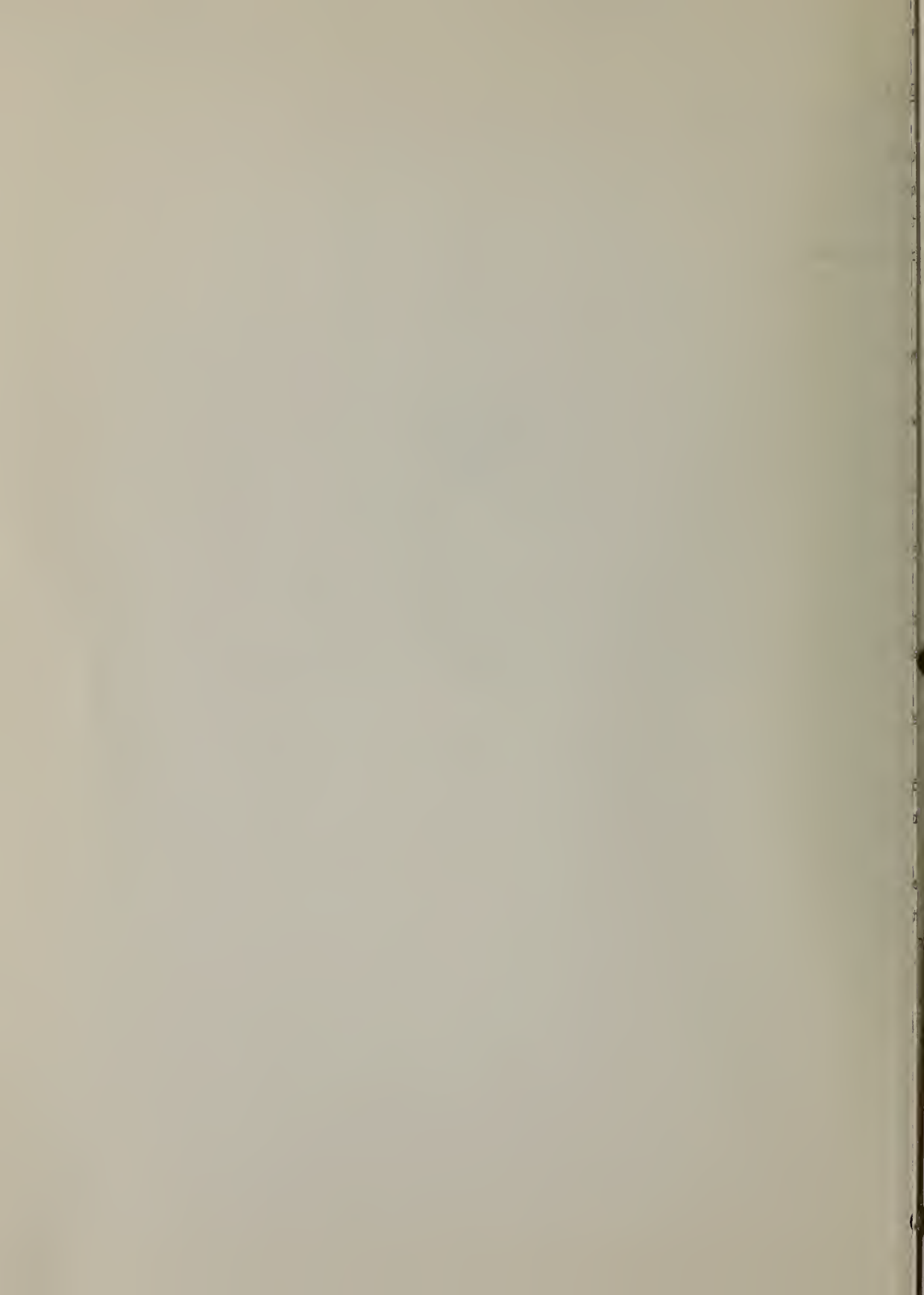
column 3 → 4	Row dimension of matrix (integer)
8 → 9	Column dimension of matrix (integer)
13 → 14	Row of first matrix element on card (integer)
18 → 19	Column of first matrix element on card (integer)
21 → 32	Values of consecutive matrix elements (row-wise) in E Format. (Blank is interpreted as zero).
34 → 45	
47 → 58	
60 → 71	

Termination of matrix input is indicated by a card with

"26" in column 3 → 4.

SECTION IV

OUTPUT



OUTPUT

Routine printout is produced for every problem deck submitted to SAAM. Special printout is added, where needed, for certain model types. Optional output is also available at the users request. This includes punched as well as printed output.

Routine printout includes:

1. A listing of the problem deck with each card printed as reformatted by SAAM.
2. SAAMs reorganization of the information in the problem deck.
3. Parameter values and a table of the initial solution values. (Zeroth iteration)
4. Results for each iteration associated with the fitting of the data.
5. Final results which include parameter values and the corresponding solution table for the "best fit" with estimated standard errors, and correlation coefficients.

Optional printout includes items requested under OPTIONS entries (card 4).

Routine and optional outputs are described in greater detail under each of the printout headings. These are given below in alphabetic order.

Special outputs in connection with particular model types are described separately at the end under the appropriate model type or subroutine.

A MATRIX BEFORE INVERSION - contains four partitions as shown below. Partition I contains coefficients $A(I,J)$ of normal equations for lambdas only, $A * RES = CR$. Partition IV contains the matrix for normal equations to calculate sigmas and kappas

I	II
III	IV

Partition II contains matrix of coefficients $\partial\sigma/\partial\lambda$ and $\partial\kappa/\partial\lambda$. Partition III contains zeroes.

Option: Column 5, card 4

$C(I)$ - denotes i^{th} component.

CONAB - is a scaling factor for the RES vector to achieve a lower sum of squares. The value of CONAB indicates the factor by which the calculated correction vector for the adjustable lambdas is multiplied.

CORRECTED SUM OF SQUARES OF PREVIOUS ITERATION. - Whenever statistical constraints are given, their statistical weights are renormalized in each iteration. To compare the sums of squares of two iterations--as a test of convergence--the sum of squares of a previous iteration is recomputed with weights assigned in the current iteration.

CORRECTIONS FOR ADJUSTABLE LAMBDA - lists the RES vector as it will be used in the current iteration. The order is that of the adjustable lambdas.

CORRELATION COEFFICIENTS - the matrix of correlation coefficients for lambdas, sigmas and kappas is partitioned as follows:

λ 's	0
0	σ 's and κ 's

The adjustable parameters appear within each partition as ordered under PARAMETERS but with the Lambdas first, then Sigmas, then Kappas.

COVARIANCE MATRIX - covariances for lambdas, sigmas and kappas. Printout is partitioned as follows:

covariance matrix of lambdas	0
0	covariance matrix of sigmas and kappas

Option: column 2, card 4

CR VECTOR - vector elements CR(I) of normal equations $A * RES = CR$
Option: column 5, card 4

D - the internal order of data, is given as the first column of the solution table. Data are ordered by t values within each block delineated by t-interrupt control cards.

FINAL VALUES - full printout of values for the "best fit" arrived at in the run. Included is a table of dependent and adjustable parameters with their estimated standard and fractional deviations, and the matrix of correlation coefficients.

INFORMATION CONNECTED WITH CALCULATION AND MODIFICATION OF RES - the RES vector as solved for from the normal equations is modified and values connected with this modification are printed in table form. (Intended as an aid in the program development).

INITIAL CONDITIONS - is a table that gives, for each component (C(I)), the F(I,0), the type of component (JUDY(I)), the changes in F(I,t) at the t-interrupt (QP(I)), and the vectors V(I) and U(I) as specified by the problem deck.

JUDY(I) - is a code that defines the type of component. JUDY(I) = 1 means that component I is a function $f_1(t)$. The code "2" signifies a summing component.

K - represents Kappa

LITTLE A BEFORE MODIFICATION - is the triangular matrix a derived from the normal equations matrix A:

$$a^T a = A$$

Option: column 5, card 4.

LITTLE A-INVERSE BEFORE MODIFICATION - is the inverse of "LITTLE A", a^{-1} , derived from the normal equations matrix A

$$a^T a = A$$

Option: column 2, card 4.

PARTIALS OF DATA POINTS WITH RESPECT TO ADJUSTABLE LAMBDA - lists, in the first two columns of the table, the component number and t-value of a datum. The remaining columns, following the order of the adjustable lambdas, list $\partial q_k(t) / \partial \lambda_j$. Each datum is given in the order in which it is stored internally. Partial derivatives for statistical constraints follow partials for the data.

Option: column 3, card 4.

PARTIALS OF SUM OF SQUARES WITH RESPECT TO ADJUSTABLE PARAMETERS -

TOTAL SS - gives the partial of the sum of squares for all the components with respect to each adjustable parameter.

FOR COMPONENT SS - gives the matrix of the partial of the sum of squares for each component with respect to each adjustable parameter. The rows correspond to the parameters and the columns to the components.

Option: column 3, card 4.

PLOT - a semi-logarithmic or arithmetic plot of the calculated and observed data. Each component which has three or more data points is plotted unless all points have identical values. In the case of the semi-log plot a) negative values will result in a diagnostic and no plot, b) off scale values are displaced by multiples of two decades to bring them onto the plot. If calculated and observed values are unequally cycled, a C is printed at the top of the graph. An asterisk, printed next to the "t" value, indicates that the scale has been stretched at that point to separate two data, with different t values, but which would have printed on top of each other because of the limited resolution. An integer, printed at the top of the graph, records the number of data plotted at the same "t" value when it exceeds one.

The symbol "+" in the plot indicates a calculated datum. The symbol "*" in the plot indicates an observed datum. The symbol "x" indicates both calculated and observed data having the same "print" value. It should be recognized that the plot has limited resolution, defined by the separation of consecutive spacings in the printer. For the semi-log plot the resolution is about 3 percent.

Option: column 4, card 4

QO(I) - represents $q_1^0(t)$

QC(I) - represents $q_1(t)$

QP(I) AT X - is the value that will replace or be added to the current value of $F(I,T)$ as instructed by the t-interrupt control card, when $t = X$.

REORGANIZED PROBLEM INFORMATION - includes:

- 1) the version of SAAM used, the number of components specified for the model, and the number of data points.
- 2) an expanded list of the data with modifications called for by control cards and with normalized statistical weights.
- 3) the initial conditions of the problem, $F(I,0)$, changes in $F(I)$ at t-interrupts, $JUDY(I)$, $V(I)$ and $U(I)$.
- 4) the parameter values listed as adjustable, dependent, fixed. Minima and maxima are given for adjustable parameters. Relations of dependent parameters are expressed in terms of non-dependent parameters.
- 5) statistical constraints and f-dependence, as interpreted by SAAM.
- 6) special output as called for.

RUNNING TIME = X - gives the time (in computer clock units) it took to run the problem.

Option: column 1, card 1

SIG - is the mean weighted variance of the data. The initial estimate of its value is made from the information in the input deck. Subsequent values are based on the solutions.

SOLUTION - the first solution is considered the zero-th iteration and is based on the set of parameters initially given. A new list of parameter values is given for each t-interrupt if the values change. Included in the output are:

- 1) the model code
- 2) SIG as estimated from the input
- 3) λ_{jj} values based on the initial parameter values

$$(\lambda_{jj} = - \sum_{i \neq j} \lambda_{ij})$$

4) a table of calculated results with headings for D (the datum number), C (the component number), t, $q_k(t)/\kappa$, κ , $q_k(t)$, $q_k^0(t)$, $(q_k^0(t) - q_k(t))$ and $q_k(t)/q_k^0(t)$.

5) a weighted sum of squares for all the data, for each COMP and for the block of statistical constraints.

5) SIG

STARTING TIME = X - gives the clock reading at the start of a problem.

Option: column 1, card 1.

TOTAL RES FOR ITERATION - the total adjustment to lambdas made during an iteration.

PUNCHED OUTPUT

A-MATRIX - the diagonal and upper half of the A-matrix for adjustable lambdas is punched out. The form used is that described under matrix entry format in the input section.

Option: column 5, card 4

COVARIANCE MATRIX - the diagonal and upper half of the covariance matrix for adjustable lambdas are punched out in matrix entry format.

Option: column 2, card 4.

CR-VECTOR - the right side of the noraml equations for adjustable lambdas is punched out as the first row of a matrix, in the matrix entry format.

Option: column 2 or 5, card 4.

MATRIX CODE CARD- one of these cards is punched out preceding an A-MATRIX or COVARIANCE MATRIX

column 1 → 10 integer portion of problem number

column 11 → 20 code for type of matrix

"1" for COVARIANCE MATRIX

"3" for A-MATRIX

column 21 → 35 the value of SIG

SECTION V
DIAGNOSTICS

DIAGNOSTICS.

The program contains a large number of internal checks which may result in diagnostic printout. If the problem calculation terminates because of a diagnostic, the program automatically proceeds to the next problem. This section contains an alphabetic listing of the diagnostics. Those that cause termination are marked with an (H). The number of the subroutine that produces the diagnostic is listed at the right. Sometimes a single input error produces multiple diagnostics.

A SUBSCRIPT (I) OF PARAMETER (J) IS INCORRECT.	(H)	1
The subscript may not be greater than the number of components in the problem.		
ADDING LAMBDA (O,J) HAS EXCEEDED LIMIT OF I.	(H)	8
A λ_{oj} is added to the parameter list for every component that does not have a λ_{oj} read in.		
ADDITIONS TO INIT. COND. NOT PERMITTED.	(H)	147
The <u>codes</u> entered as initial conditions cannot be changed at a t-interrupt. Model Code 18.		
ALL VALUES IN COMPARTMENT I ARE NEGATIVE. LOG PLOT IS IMPOSSIBLE.		84
ALL WEIGHTS = 1.	(H)	2
No weights were assigned to the data and the program has assigned a weight of 1. to each datum and set the number of iterations to zero.		
ALL WEIGHTS FOR COMPONENT (I) ARE ZERO, THEREFORE KAPPA (I) CANNOT BE VARIABLE.	(H)	19
An adjustable kappa cannot be calculated for a component if all data for that component have zero statistical weight.		
AMT. COMP. I SET = $\pm 10.E12$		46
An amount calculated for component I has been set at $\pm 10^{12}$ in order to avoid overflow or underflow on the computer (i.e. the calculated value was outside the limit set at $\pm 10^{12}$). Model codes 1 and 4		
AT MATRIX OVERFLOW.	(H)	97
The storage of information has exceeded the available storage locations. Model Code 3.		
AT-MATRIX OVERFLOW.	(H)	98
Matrices and related information have exceeded the available storage. Model Code 11.		
AT-MATRIX OVERFLOW. ITER. SET TO ZERO		135
Storage space for added matrix is insufficient. Only the initial solution is made, and without the matrix information.		

- AT T = X EXPONENTIAL LIMITED TO E**30. 39
 The amount calculated at $t = X$ exceeded e^{30} ,
 a limit set in the program. The amount is set
 at e^{30} and the problem continued. Model Code 9.
- AT T = X LAMBDA (I,J)* Y SET = 1.069 E 13 56
 An exponent, λt , has exceeded 30. and been set
 equal to 30. Model code 2.
- AT T = X LAMBDA (I,2) = Y 148
 The Gaussian function called for cannot be
 calculated and $f_i(t)$ for that value of t
 remains zero. Model Code 18.
- CODE INCORRECT FOR F(I). (H) 147
 The request for calculations as entered under the
 initial conditions heading includes an incorrect
 component number or operational code. Model Code 18.
- COMP (I) ISOLATED FOR STEADY STATE CALC. SINCE $L(I,I) = 0$. 57
 COMPONENT (I) NOT IN MODEL BUT INITIAL CONDITION GIVEN. (H) 9
 The component named under the initial conditions
 heading has an index greater than the highest
 index in the model.
- COMPONENT NUMBER (L) FOR DATUM (I) EXCEEDS N. (H) 2
 A data point has been entered for compartment L,
 $L > N$, the number of components specified for
 the problem.
- COVARIANCE MATRIX IRREGULAR 41
 Negative diagonal elements resulting from
 inversion of ill-conditioned matrices may
 cause this diagnostic.
- DATA DELETED FOR T = X 68
 The data for t given by the diagnostic is incomplete
 and the point has been dropped from the data list
 in the solution. Model Code 5.

DATA EXCEED I.	(H)	2
I is the limit for number of data entries.		
DATA INCOMPLETE		68
Some information in the data list is missing.		
A complete set of observations must be entered as data at each <u>t</u> . Model Code 5.		
DATA INDIV. I INCOMPLETE.	(H)	98
Data giving the values for individual I are missing. Model Code 11.		
DATA INSUFFICIENT.	(H)	68
There are not enough data given (correctly) to continue the solution. Model Code 5.		
DATA PLUS STATISTICAL CONSTRAINTS EXCEED I.	(H)	7
The number of data entries <u>plus</u> the number of statistical constraints is limited to a maximum of I.		
DATA STORAGE EXCEEDED.	(H)	97
Information is stored jointly with the partials matrix. This diagnostic results when the space is insufficient to store all the information given. Model Code 3.		
DEGREES OF FREEDOM LESS THAN 3.	(H)	4
The number of weighted data points minus the number of adjustable lambdas is less than 3.		
The solution will proceed if an estimate of SIG exists.		
DEPENDENCE DIAGNOSTIC. NO PARAMETER (I,J) IN LIST.	(H)	6
The dependence relations include a parameter which is not in the parameter list.		
DEPENDENCE DIAGNOSTIC. PARAMETER (I,J) IS NOT DEPENDENT BUT DEPENDENCE IS GIVEN.	(H)	6
DEPENDENCE MATRIX IS SINGULAR.	(H)	11
Insufficient (or incorrect) dependence relations were entered.		

DEPENDENCE ON PARAMETER (I,J) HAS BEEN ENTERED TWICE.	(H)	6
A single constraint has two terms involving parameter (I,J).		
DEPENDENT PARAMETER (I) UNDEFINED.	(H)	11
Give dependence relation for the I th parameter		
DIVIDING BY 0.	(H)	109
Model Code 13.		
ENTRY CONTROL CARDS INCOMPATIBLE.	(H)	2
Relative weights for some of the data points cannot be combined with absolute weights for other data points.		
ERROR IN MATRIX READ-IN.	(H)	135
The matrix supplied as additional information under special options (card 2) has been punched incorrectly.		
ESTIMATE OF ABSOLUTE DEVIATION OF DATA NEEDED.	(H)	19
The degrees of freedom are less than 3 and calculation cannot proceed without additional information		
EXCESS DEPENDENTS = I.	(H)	11
There are I more dependent parameters than storage will allow.		
F(I) CODES ILL-DEFINED.	(H)	147
The codes entered under initial conditions are in question. Model Code 18.		
F(I) = 0. F(J) NOT COMPUTED.		147
The calculation of F(J) is omitted (it is set to zero) since it requires division by F(I) which is zero. Model Code 18.		
FUNCTION INPUT ERROR.	(H)	97
Model Code 3.		
FUNCTION X NOT IN DATA.	(H)	97
Model Code 3.		
GIVE DEPENDENCE RELATION FOR PARAMETER (I,J).	(H)	6

- HALT DIVIDING BY ZERO. (H) 108
 Model Code 12.
- INITIAL CONDITIONS GIVEN FOR SUMMING COMPONENT (J). (H) 5
 Initial conditions may not be given for a summing component.
- INITIAL CONDITIONS NEEDED. (H) 27
 See requirement under Model Code used.
- INITIAL ESTIMATE LAMBDA (I,J) OUTSIDE LIMIT. ITERATIONS SET TO ZERO. (H) 4
 An upper or lower limit for λ_{ij} is violated by the initial estimate of the value of λ_{ij} . A zero iteration calculation is performed and the problem is halted.
- JJ CALCULATION EXCEEDS STORAGE. (H) 11
 The information for λ_{jj} calculation is stored in the dependence matrix and has exceeded the space available. This can be corrected by reducing the number of dependent parameters and/or, if some component numbers have been skipped, renumbering to reduce the total number of components.
- KAPPA (I) CANNOT BE VARIABLE BECAUSE ALL SIGMAS INTO SUMMER (I) ARE NOT FIXED. (H) 12
 Either κ_i or σ_{ji} must be fixed to permit solution of the model.
- $L(I,I) = 0$. C(I) ISOLATED FROM SYSTEM FOR CALC. 141
 Component (I) cannot be included for steady state calculations. Model Code 16.
- LAMBDA (I,I) = 0. COMP. (I) ISOLATED FROM SYSTEM FOR CALCULATION OF U OR V. 42
 In the calculation of steady state values component (I) cannot be included in the system.
- LAMBDA (I,0) UNDEFINED. (H) 4
 The second subscript of a lambda cannot be zero.

LAMBDA MATRIX SINGULAR.	(H)	141
The matrix of lambdas cannot be inverted		
Model Code 16.		
LAMBDA (0,1) NEEDED.	(H)	104
Model Code 10.		
LAMBDA INCORRECT.	(H)	98
Lambda (0,1) must be entered for each component.		
Model Code 11.		
LIMITS PARAMETER (I,J) INCORRECT.	(H)	1
Lower limit higher than upper limit?		
MATRIX I.D. FOR INDIV. I INCOMPLETE.	(H)	98
The information on the card preceding a matrix		
has one or more entries missing. Model Code 11.		
MATRIX INPUT ERROR.	(H)	97
The matrix input is incorrectly punched.		
Model Code 3.		
MATRIX INPUT INCORRECT.	(H)	103
The matrix reading routine has found the matrix		
dimensions, as punched, incompatible either		
with the dimensions of the matrix required by		
the problem, or with the subscripts of a matrix		
entry, as punched.		
MATRIX N.G. FOR I.	(H)	98
The matrix input for individual I, is		
incorrectly punched. Model Code 11.		
MATRIX SINGULAR.	(H)	57
The matrix used in the solution is singular.		
Model Code 3.		
MODEL NOT SUITABLE FOR ANALYTIC SOLUTION.	(H)	17
The model requires the use of the		
differential equations solution, model types 1 or 4.		
NO ADJUSTABLE LAMBDA. ITERATIONS SET TO ZERO.		19
If there are no adjustable lambdas the number		
of iterations is set to zero.		
NO ADJUSTABLE PARAMETERS.		67

NO PARAMETER (I,J) IN LIST BUT STATISTICAL CONSTRAINT GIVEN.	(H)	7
Parameter (I,J) entered in a statistical constraint, is not in the list of parameters.		
NO. OF ADJUSTABLE PARAMETERS EXCEEDS I.	(H)	5
NO. OF DEPENDENTS EXCEEDS I.	(H)	1
NO. OF PARAMETERS EXCEEDS I.	(H)	1
NO. OF STEPS NEG. FOR CALC. OF DATUM I.	(H)	21
An inconsistent t-interrupt entry has probably resulted in a negative t increment.		
OVERFLOW COMPUTING F(I) AT T = X.		147
The solution in progress is completed and the problem is terminated. Model Code 18.		
OVERFLOW IN COMP. I AT T = X.	(H)	109
Model Code 13.		
PARAMETER DEPENDENCE ON C(I) INCORRECT.	(H)	1
I probably exceeds the highest component index.		
PARAMETERS I AND J ARE DUPLICATES.	(H)	19
A parameter has been entered twice in the input data.		
PARAMETER I = X, NOT PUNCHED.		136
The limits of the floating point field were insufficient to accommodate the parameter value.		
PARTITION I OF THE MATRIX IS SINGULAR. THE FOLLOWING ADJUSTABLE PARAMETERS ARE INVOLVED.	(H)	44
Symmetric matrices are partitioned into independent blocks for inversion. A partition involving the listed parameters is singular. At least one of the parameters in this block is dependent.		
RATIO OF CALCULATED SIGMA TO ESTIMATED SIG = X, ITERATIONS SET TO ZERO		29
The deviation of the calculated from the observed values is more than ten times greater than implied by the input estimate of the errors. Better initial estimates of parameters or larger estimates of standard deviations of data are needed.		

SIG = 0. RES. NOT MODIFIED		134
The RES vector resulting from solution of the normal equations could not be modified because SIG = 0., and modification includes a calculation requiring division by SIG. The solution continues with the unmodified RES.		
SIGMA - KAPPA MATRIX IS SINGULAR.		23
The matrix of coefficients of the normal equations used to calculate σ 's and κ 's is singular		
SIGMA KAPPA MATRIX SINGULAR.	(H)	34
The matrix of normal equations for the solution of sigmas and/or kappas is singular.		
SPREAD OF VALUES FOR COMPARTMENT I EQUALS ZERO.		84
Plot will be omitted.		
SQUARE ROOT UNDEFINED.	(H)	108
The result of the calculation would be an imaginary number. Model Code 12.		
STD. DEVS. FOR I GIVEN WITH MATRIX FOR J.	(H)	98
STORAGE OVERFLOW.	(H)	147
The available storage is insufficient for the calculation of codes submitted. It may be possible to simplify the input to fit within available storage. Model Code 18.		
T, AT T-INTERRUPT I EXCEEDED BY DATUM J.	(H)	2
The T value of datum (J), in the block terminated by T-interrupt card (I), exceeds the T value of the T-interrupt.		
T-INTERRUPT DIAGNOSTIC. A COMPONENT NO. EXCEEDS N.	(H)	32
The subscript of a t-interrupt entry exceeds the number of components in the model.		
T-INTERRUPT DIAGNOSTIC. PARAMETER (I,J) OR PARAMETER (K,L)		
NOT IN LIST.	(H)	32
A parameter to be changed at a t-interrupt is not in the original parameter list.		

T-INTERRUPTS EXCEED I. (H) 2
I is the maximum number of t-interrupts permitted.

THE LAMBDA MATRIX IS SINGULAR 42
In the calculation of compartment sizes, V, the λ matrix is singular. Model Code 1.

TIME ALLOWED EXCEEDED AT T = XX. INCREASE TIME FACTOR
IF DESIRED. (H) 21
Program estimates computation time and limits computations to a preset internal reference. This can be changed by a Time Factor entry on card 3.

TOO FEW STEADY STATE EQUATIONS. (H) 97
The number of equations must be equal to the number of components. Model Code 3.

TOO MANY COMPONENTS IN MODEL. (H) 2

TOO MANY KAPPAS LISTED. (H) 3

TOO MANY STEADY STATE EQUATIONS. (H) 97
The number of equations must be equal to the number of components. Model Code 3.

V AND U MAY NOT BOTH BE GIVEN. 42
No compartment sizes (V) may be given if any steady state inflow rates (U) are given, and vice versa. Model Code 1.

VALID ONLY FOR NON-SUMMERS. 14
Information already available in storage is printed out but is valid only for the f_i of the model.

VARIANCE NEGATIVE 69
A standard deviation cannot be calculated because a diagonal element of the covariance matrix is negative.

VARIANCE NEGATIVE, S. D. SET TO ZERO 42
A diagonal element of the covariance matrix is negative and its square root (the standard deviation) cannot be calculated.

WEIGHTS FOR COMPONENT (I) ARE ZERO THEREFORE

SIGMA (J,I) CANNOT BE ADJUSTABLE. (H) 19

An adjustable sigma cannot be calculated if the data for the summer component have zero statistical weight.

ZERO DIAGONAL ELEMENTS MATRIX IS SINGULAR (H) 44

One or more diagonal elements of the symmetric matrix being inverted are zero.

ZERO DIVISION IN COMP. I. $T = X$ 45

Calculation of the I^{th} component called for division by zero at the point whose T value is X. Model Code 7.

SECTION VI

MODEL TYPES

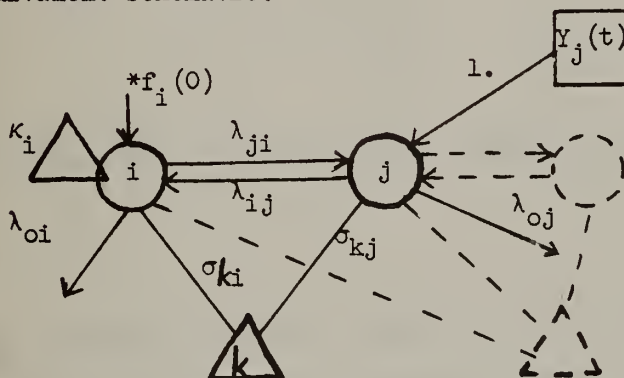
Model Types1. Linear differential equations with constant coefficients:

$$\frac{df_j(t)}{dt} = \sum_{\substack{i=1 \\ i \neq j}}^n \lambda_{ji} f_i(t) - \sum_{\substack{i=0 \\ i \neq j}}^n \lambda_{ij} f_j(t) + Y_j(t)$$

Initial conditions: $f_j(0)$

$$q_k(t) = \kappa_k \sum_{j \neq k} \sigma_{kj} f_j(t) \quad \text{or} \quad q_i(t) = \kappa_i f_i(t)$$

The λ_{ij} are time independent. $Y_j(t)$ is an arbitrary input function into j . Equivalent schematic:



Computational procedure.

The differential equations are solved using a 4th order

Runge-Kutta method.

In addition and independently of the above solution, a steady state solution V can also be obtained from a constant input vector U , entered separately. In matrix notation this is given as

$$V = \lambda^{-1} U$$

or

$$U = \lambda V$$

where U and V are vectors and λ is the matrix of coefficients:

$$\lambda = \begin{vmatrix} \lambda_{11} & -\lambda_{12} & -\lambda_{13} & \dots \\ -\lambda_{21} & \lambda_{22} & -\lambda_{23} & \\ -\lambda_{31} & -\lambda_{32} & \lambda_{33} & \\ \vdots & \vdots & \vdots & \vdots \end{vmatrix}$$

At present these calculated values cannot be fitted against observed values.

Special Inputs:

Card 4: enter "1" under MODEL CODE. This entry may be left blank, in which case the program will try to use model code 2, if the problem meets the requirements for that model code. If not, it will use model code 1.

Initial conditions: enter initial conditions for differential equations, $f_i(0)$, under INITIAL CONDITIONS.

Enter either the vector V or the vector U in their appropriate fields, if a steady state solution is desired. When an entry U_1 (or V_1) is omitted it is automatically set to zero by the program.

Special Outputs:

INVERTED LAMBDA MATRIX (Option).

U(I), V(I) and R(I,J), when steady state solutions are requested.

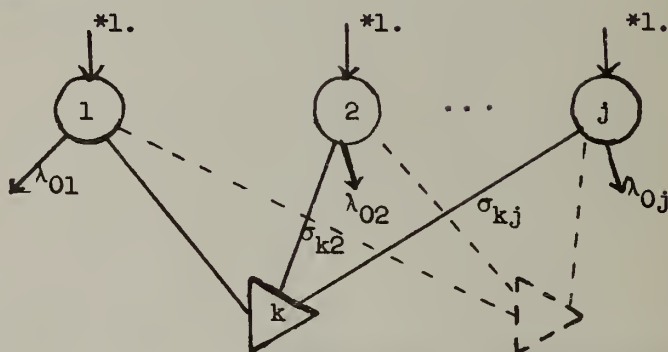
$$R(I,J) \equiv \lambda(I,J)*V(J)$$

2. Sums of Exponentials

$$f_j = e^{-\lambda_{0j}t}$$

$$q_k = \kappa_k \sum \sigma_{ki} f_j(t) \quad \text{or } q_1 = \kappa_1 f_1(t)$$

Equivalent schematic



Computational procedure:

Evaluation of $e^{-\lambda_{0j}t}$ for each datum

Model code: 2 (column 50, card 4)

User may leave code "blank" in which case program will choose model code 2 if it can, or else it will choose either model code 1 or 4, whichever is appropriate.

3. Similarity Transformation (MAPPING)

This SOLVE routine performs a similarity transformation on a given matrix M:

$$F = \lambda M \lambda^{-1}$$

F, λ and M are $n \times n$ matrices.

Option A:

$$f_1(t_{ij}) = F(I, J) \quad I = 0, 1, \dots, n$$

$$J = 1, 2, \dots, n$$

where $F(I, J)$ is the I^{th} row and J^{th} column element of the matrix F for $I \neq 0$, and $F(0, J) = \sum_{I=1}^n F(I, J)$

$$f_2(t_{ui}) = U(I)$$

$$f_2(t_{vi}) = V(I)$$

where $U(I)$ and $V(I)$ are solutions of the simultaneous set of $2n$ linear equations

$$\begin{cases} \sum_{J=1}^n F(I, J) V(J) - U(I) = 0 & I = 1, 2, \dots, n \\ \sum_{K=1}^n A(I, K) V(K) + \sum_{M=1}^n B(I, M) U(M) = C(I) & I = 1, 2, \dots, n \end{cases}$$

$A(I, K)$, $B(I, M)$ and $C(I)$ are required for the calculation of $U(I)$ and $V(I)$ and are entered by the user under special input described later.

$$f_2(t_{rij}) = R(I, J)$$

where $R(I, J) = f_1(t_{ij}) \cdot V(J)$. The $R(I, J)$ are calculated after $V(J)$ are determined.

$$f_2(t_{xi}) = X(I)$$

$$\text{where } X(I) = \sum_K D(I, K)V(K) + \sum_J E(I, J)U(J)$$

$D(I, K)$ and $E(I, J)$ are entered as special input described later. The $X(I)$ are calculated after the $V(K)$ and $U(J)$ are determined.

Option B

$$\begin{aligned} f_1(t_{ij}) &= -F(I, J) && \text{for } I \neq J \text{ and } I \neq 0 \\ &= F(I, J) && \text{for } I = J \text{ and } I = 0 \end{aligned}$$

$$\left. \begin{aligned} f_2(t_{ui}) \\ f_2(t_{vi}) \end{aligned} \right\} \text{ same as option A}$$

$$f_2(t_{rij}) = f_1(t_{ij})V(J)$$

$$f_2(t_{xi}) \text{ same as option A}$$

(Note: In linear compartmental systems with constant coefficients U , V , R and X are steady state quantities).

Special inputs:

Card 2: "n" (dimension of $F(I, J)$) under NO OF COMPONENTS.

Card 4: "3" under MODEL CODE

Column 70

$$\left\{ \begin{array}{ll} \text{"1"} & \text{Option A} \\ \text{Blank} & \text{Option B} \end{array} \right.$$

Data:

COMP NO.: "1." for f_1 "2." for f_2

T: I + .01*J for F(I,J) [e.g. 1.02 for F(1,2)]
 30. + .01*I for V(I) [e.g. 30.11 for V(11)]
 60. + .01*I for U(I) [e.g. 60.02 for U(2)]
 100. + I + .01*J for R(I,J) [e.g. 101.02 for R(1,2)]
 150. + .01*I for X(I) [e.g. 150.12 X(12)]

Initial Conditions:

No entries needed except when $f_2(t)$ computations are called for,
 in which case enter a "1." in columns (42 → 55) of the "26"
termination card for this block.

Lambdas:

Elements of $\lambda(I,J)$ matrix

Special:

Matrix M is entered after last "26" termination card of regular
 data deck. The format is as given in Section III 28. Each
 matrix is terminated by a card with "26" in column 3 → 4.

The constants A(I,K), B(I,M) and C(I) involved in the equations for
U and V:

$$\sum_K A(I,K) V(K) + \sum_M B(I,M) U(M) = C(I)$$

are entered after the matrix M block, one card for each term of
 the equation in the following format:

column 4 → 5 enter 30 for V(K), 60 for U(M) (integer)

column 9 → 10 enter K or M (integer)

column 13 → 25 enter A(I,K) or B(I,M) (decimal)

On the card containing the last term of each equation make the additional entries:

column 26 "="

column 27 → 40 enter C(I) (decimal)

The program requires that n equations be entered. The entire set of equations is terminated by a card with a "26" in column 4 → 5.

The constants D(I,K) and E(I,J) involved in the equations for X:

$$X(I) = \sum_K D(I,K) V(K) + \sum_J E(I,J) U(J)$$

are entered next under the following format, one card for each term:

column 3 → 5 enter "150 (integer)

column 9 → 10 enter I (integer)

column 19 → 20 "30" for V(K), "60" for U(J) (integer)

column 24 → 25 enter K or J (integer)

column 27 → 40 enter D(I,J) or E(I,J) (decimal)

The entire set of X(I) entries are terminated by a "26" in column 4 → 5. The X(I) values are entered under Data as described earlier.

Special outputs

LAMBDA MATRIX - is the matrix λ to be used to solve the equations

$$FV = U.$$

LAMBDA-INVERSE MATRIX - is the inverse of the lambda matrix.

MATRIX - is the matrix, M , given in the input for solution of the

$$\text{equations } F = \lambda M \lambda^{-1}.$$

STEADY STATE EQUATIONS - are linear equations in U and V to be

solved given the matrix of λ 's

STEADY STATE FUNCTIONS - are additional constraints in U and V .

4. Ordinary non-linear differential equations

$$\left. \begin{aligned} \frac{df_j}{dt} &= \sum_{\substack{i=1 \\ i \neq j}}^n \lambda'_{ji} f_i(t) - \sum_{\substack{i=0 \\ i \neq j}}^n \lambda'_{ij} f_j(t) + Y_j(t) \end{aligned} \right\} j = 1, \dots, n$$

initial conditions: $f_j(0)$

$$q_k(t) = \kappa_k \sum_{j \neq k} \sigma'_{kj} f_j(t) \quad \text{or} \quad q_i(t) = \kappa'_i f_i(t)$$

$$q_k(t) = \kappa'_k \sum_{j \neq k} \sigma_{kj} f_j(t)$$

The parameters designated by a 'prime' can be f -dependent.

For example, let

$$\frac{df_1}{dt} = \lambda'_{12} f_2 - \lambda'_{21} f_1 + \lambda'_{31} f_1 + \lambda'_{13} f_3$$

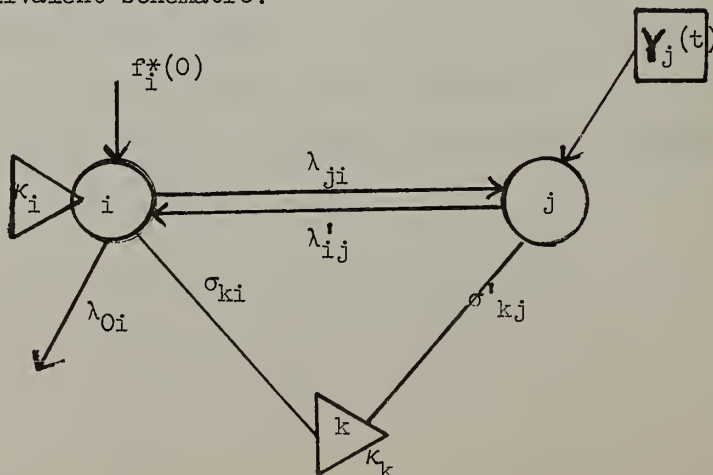
If $\lambda'_{12} = \lambda_{12} f_h$, $\lambda'_{21} = \lambda_{21}/f_j$, $\lambda'_{31} = \lambda_{31}/f_i$, $\lambda'_{13} = \lambda_{13}$, then

$$\frac{df_1}{dt} = \lambda_{12} f_h f_2 - \lambda_{21} f_1 / f_j + \lambda_{31} + \lambda_{13} f_3$$

Similarly, if $q_7 = \kappa_7 f_7$ and $\kappa'_7 = \kappa_7 / f_6$, then $q_7 = \kappa_7 f_7 / f_6$

$Y_j(t)$ is an arbitrary input function into j .

Equivalent schematic:



Computational procedure:

4th order Runge-Kutta method is used for solution of differential equations.

Special inputs:

Card 4 - enter "4" under MODEL CODE. If this entry is blank the program will appropriately choose between models 1, 2, or 4.

λ 's σ 's, κ 's--enter f-dependence information in columns 57 \rightarrow 59.

Special outputs:

In case of interruptions in solution special intermediate results are printed.

5. Linear Combination of Spectra

$$f_j(t_k) = \bar{f}_j(t_k + \lambda_{j1}) \quad j = 2, 3, \dots$$

where $\bar{f}_j(t_k)$ are given values for spectrum j at t_k and

λ_{j1} is some arbitrary t shift in the coordinate system for f_j .

$$q_k(t_k) = \sum_{\substack{j=2 \\ j \neq k}}^n \sigma_{kj} f_j(t_k) \quad k = 2, 3, \dots$$

Computational procedure: linear regression

Special inputs:

Card 4: enter "5" under MODEL CODE

Data: COMPONENT - index j of f_j

T - value of t_k . Every function $f_j(t_k + \lambda_{j1})$ must have a value at each t_k .

OBSERVED VALUE - $\bar{f}_j(t_k + \lambda_{j1})$ and $q_k(t_k)$ values

θ - derivative of $f_j(t_k + \lambda_{j1})$, if available.

6. Sum of Gaussians and Exponentials

$$f_j(t) = \frac{e^{-(t-\lambda_{j1})^2/2\lambda_{j2}^2}}{\sqrt{2\pi} \lambda_{j2}} \quad \text{for } j > 3$$

$$f_h(t) = e^{-\lambda_{h3}t} \quad \text{for } h > 3$$

$$q_k(t) = \kappa_k \sum_{i \neq k} \sigma_{ki} f_i(t) \quad \begin{array}{l} i > 3 \\ k > 3 \end{array}$$

Special input:

Card 4 - "6" under MODEL TYPE

7. Population Survival Function

$$f_j(t) = f_j(0) e^{-\lambda_j t} [1 - (1 - e^{-\lambda_j t})^{\lambda_j}] \quad \text{for } j > 3$$

$$q_k(t) = \kappa_k \sum_{j \neq k} \sigma_{kj} f_j(t) \quad \text{for } k > 3$$

Special input:

Card 4 - "7" under MODEL CODE

8. Power Series

$$f_j(t) = t^j \quad \text{for } j = 1, 2, \dots, m$$

$$f_{m+1}(t) = 1.$$

$$q_k(t) = \kappa_k \sum_{\substack{j=1 \\ j \neq k}}^{m+1} \sigma_{kj} f_j(t) \quad \text{for } k > (m+1)$$

Special inputs

Card 4 - "8" under MODEL CODE

"m" in column 70

9. Special Function

$$f_j(t, \theta) = (1 + \lambda_{j1}\theta) e^{-\lambda_{j2}t(1 - \lambda_{j3}\theta)} \quad j > 3$$

$$q_k(t, \theta) = \kappa_k \sum_{j \neq k} \sigma_{kj} f_j(t, \theta) \quad k > 3$$

Special inputs:

Card 4 - "9" under MODEL CODE

11. Population Mean and Covariance Matrix

Purpose: Given a population of k studies in which each study i contains a set of n parameters with values X_i ($X_{i1}, X_{i2}, \dots, X_{in}$) and covariance matrix V_i , find the mean parameter values \bar{X} ($\bar{X}_1, \bar{X}_2, \dots, \bar{X}_n$) and the covariance matrix (\bar{V}) for the population.

Solution equations: the program solves the following set of simultaneous equations, approximately

$$\bar{X} = \left[\sum_i (V_i + \bar{V})^{-1} \right]^{-1} \left[\sum_i (V_i + \bar{V})^{-1} X_i \right]$$

$$\bar{v}_{lm} = \frac{1}{k-1} \sum_i \sqrt{\omega_{il} \omega_{im}} (X_{il} - \bar{X}_l) (X_{im} - \bar{X}_m)$$

where

\bar{v}_{lm} = (l, m) element of covariance matrix \bar{V}

ω_{il} = statistical weight of parameter l , study i , internally calculated.

Special inputs:

Card 2 - NUMBER OF COMPONENTS = n = number of parameters

NUMBER OF ITERATIONS: Blank

Card 4

MODEL CODE: "11"

Data (1):

COMP: Parameter number (say, j)

I: study number (2) i (any number 0. → 999.)

OBSERVED VALUE: the value of X_{ij} - parameter j in study i

WEIGHT: enter "1" directly or through control card

Lambdas:

COMP NUMBER: subscripts for λ_{oj} entered for $j = 1, \dots, n$.

No other entries are required under this format.

Additional Input:

Immediately after the standard deck the following are entered in the order indicated.

For each study⁽¹⁾:

Control card:

Columns 1 \rightarrow 10: The study number i (integer)

11 \rightarrow 20: Code (integer) for the type of matrix input which is to follow

"1" - covariance matrix

"2" - correlation coefficient matrix with standard deviations on diagonal.

"3" - normal equations matrix

"4" - normal equations matrix followed by vector of standard deviations

(Any one of the above may be used as input matrix)

21 \rightarrow 35: SIG for study i (E format).

(SIG = sum of squares of deviations divided by degrees of freedom.)

Matrix⁽³⁾: See Section III-28

Vector: Same as matrix format (Section III-2.1)

This entry is required only if called for by code entered on "control card".

Footnotes:

- (1) Punched cards for these entries can be obtained in proper format for each study i by entering a "1" under options in either columns 3 or 5, when "running" study i under its model code.
- (2) Study numbers must be different from each other in the integer portions. They are ordered internally by their integer values and assigned internal numbers from 1 \rightarrow k.
- (3) Since the matrices are symmetric, only upper-right or lower left portions (including diagonal) need be entered.

Special outputs

A-MATRIX FOR POPULATION

A-MATRIX (OPTIONAL) is the A-Matrix for an individual in the population.

Option: Column 6, Card 4.

CORRELATION COEFFICIENT MATRIX FOR POPULATION

INDIVIDUAL = I, CODE = J, SIG = X - is the code card identifying, for the matrix which follows, the problem (INDIVIDUAL), the type of matrix (CODE) and SIG. The Code is "1" for a covariance matrix, "2" for a correlation coefficient matrix with the standard deviations as diagonal elements, "3" for the A-matrix and "4" for the A-matrix followed by the vector of standard deviations.

MATRIX AS READ - is the matrix supplied to the program for an individual in the population being studied.

SIG FOR POPULATION = X - is the mean variance of the parameters for the population being studied.

VARIANCE CO-VARIANCE MATRIX FOR ADJ. POPULATION - is the covariance matrix for the population calculated after the parameters (for each individual in the population) have been adjusted toward the mean within a 95% confidence limit.

SECTION VII

COMPUTATIONAL PROCEDURES AND METHODS

The following are the computational stages in SAAM connected with the solution of a problem:

Read-in

Set-up

Solve (zeroeth iteration)

Iterate: a) Partial derivatives

b) Parameter adjustment

Final Results

Wind-up

Special

Plot

READ-IN

A problem deck consists of a number of distinct blocks, each carrying a different type of information about a problem. Some computations are intermixed with read-write instructions, but most occur after the deck is read in.

The first four cards of the problem deck are stored in core. When "clocking" is requested, the clock time at the start of a problem is stored and printed.

The DATA block is read and stored in core next. Instructions carried by the Data Control Cards are executed during the read-in.

INITIAL CONDITIONS and the KAPPAS, LAMBDA S, and SIGMA S blocks are read after the DATA.

DEPENDENCE RELATIONS are read into temporary storage. Dependent parameters are expressed in terms of independent ones (adjustable and

fixed):

$$Ax = By$$

where x is the vector of the dependent parameters and y is the vector of the independent ones. A and B are matrices of coefficients. Solution for x gives:

$$x = A^{-1} By$$

The matrix $A^{-1} B$ is stored for subsequent use.

STATISTICAL CONSTRAINTS are read, and stored jointly with the data to be used in the least squares fit.

T-INTERRUPT CHANGES IN $f_i(t)$ are read and stored in core.

T-INTERRUPT CHANGES IN PARAMETERS are stored on tape and brought into core each time they are needed.

Inputs required for special model types are read during the set-up wind-up and special computational stages of the problem solution.

Reorganization of data and parameters takes place during and after the read in. Data are rearranged, new parameters are added when required, internal codes are set up for computational control, etc. Some of the reorganized information appears in the print-out.

The input DATA are rearranged in order of increasing t within each t -interrupt block. In some model types data are added or deleted. A diagnostic usually explains deletions.

Statistical weights are assigned to the data. First, weights are assigned in accordance with the weight code. When weights are assigned to the data directly, they are entered as is. When a standard deviation (s.d.)

is assigned to a datum its weight (W) is calculated as:

$$W = \frac{1}{(\text{s.d.})^2}$$

When a fractional deviation (f.d.) is assigned to a datum, the weight (W) is calculated as

$$W = \frac{1}{[(\text{f.d.}) * q^0(t)]^2}$$

where $q^0(t)$ is the OBSERVED value for the datum. When the standard deviation (s.d.) or observed value $q^0(t)$ are zero, the weight assigned to the datum is also zero.

After weights are assigned to all data, they are normalized so that the sum of the weights equals the number of data points having non-zero weights.

Weights assigned directly to data are considered relative, whereas weights derived from standard or fractional deviations are considered absolute. The program does not permit the mixing of relative and absolute weight assignments in the input data.

When the weights are absolute, it is possible to calculate a "read-in" average variance (SIG) per datum:

$$\text{SIG}_{\text{read-in}} = (W_n)_k * (\text{s.d.})_k^2$$

where $(W_n)_k$ is the normalized weight for any datum, k, having non-zero weight.

Weights (W_c) are assigned to the statistical constraints:

$$W_c = \frac{\text{SIG}_{\text{read-in}}}{(\text{s.d.})_c^2}$$

where $(s.d.)_c$ is the standard deviation read in for the statistical constraint.

SET-UP

Computations to test and augment special information required for the particular model type are carried out here. Every model type has its own set-up routine.

SOLVE (Zeroeth Iteration)

Once the parameters, data and other entries are organized, a solution for the particular model type in the problem starts.

When a solution starts with a t-interrupt all changes in f_i and parameters are executed first. Values for the dependent parameters are then calculated from the stored dependence relations.

The solution proceeds in accordance with the equations defining the model type. $f_i(t)$ values are derived for each datum and for each of the statistical constraints.

Sigmas (and kappas) to yield a least squares fit of the data are calculated next from the linear regression equations:

$$\sum_i \sigma_{ki} f_i(t_k) = q_k^0(t_k) \quad \text{for all } k.$$

The calculated σ_{ki} , are then used to calculate $q_k(t)$. Comparison of $q_k^0(t)$ and $q_k(t)$ permits the calculation of a SIG_{calc}

$$SIG_{calc} = \sum_k \frac{[q_k^0(t) - q_k(t)]^2 w_k}{d.f.}$$

where d.f. are the degrees of freedom, the number of weighted data

points less the number of adjustable lambdas.

In subsequent computations, SIG_{calc} is used in place of $SIG_{read-in}$ if its value is lower.

Weights for statistical constraints are recalculated when the value of SIG_{calc} is lower than the value of $SIG_{read-in}$:

$$W_c = \frac{SIG_{calc}}{(s.d.)_c^2}$$

after statistical weights are reassigned, weighted sum of squares and SIG values are calculated for all data and statistical constraints.

SIG_{calc} is compared with $SIG_{read-in}$. If the ratio is greater than 100, the problem solution is terminated at the zeroeth iteration, implying that initial estimates for parameters are not good enough to continue. This termination can be overcome by improved initial estimates of parameters or by entering larger standard deviations for data. (This will not alter final least squares parameter values or their estimated uncertainties if statistical constraints are altered by the same factor)*. The latter change should only be made if convergence with poor initial estimates is possible or economical.

*Tentatively this can also be overcome by entering a large value of P on card 3. $P = 3$ is routinely used internally. $P = 10000$ would in almost every case evade the test.

ITERATIONSA. Partial Derivatives

After the zeroeth iteration, partial derivatives of the calculated $q_k(t)$ with respect to each of the adjustable lambdas are derived. The calculations are performed by numerical approximation

$$\frac{\partial q_k(t)}{\partial \lambda_{ij}} \approx \frac{\Delta q_k(t)}{\Delta \lambda_{ij}}$$

Each of the adjustable λ_{ik} is changed by a small fraction, P_1 , (Card 3) to a value $(\lambda_{ij} + P_1 * \lambda_{ij})$ and a new $q_k(t)$, designated as $q_k^p(t)$ is obtained using the procedure outlined under SOLVE. An approximation for the partials is obtained as

$$\frac{q_k^p(t) - q_k(t)}{P_1 * \lambda_{ij}}$$

The value of P_1 , normally .01, can be changed on Card 3. The recalculated $q_k^p(t)$ include readjusted sigmas and kappas, when the latter are adjustable or dependent. Partial derivatives are calculated for all data and statistical constraints.

Normal equations are derived from the matrix of partial derivatives, and an estimate for a correction vector (RES) for the adjustable λ_{ij} -- based on linear approximation theory -- is calculated:

$$RES = (a^T W a)^{-1} a^T W b$$

a is the matrix of partial derivatives, W is a diagonal matrix of the weights and b is the vector $[q_k(t) - q_k^o(t)]$.

B. Parameter Adjustment

After the correction vector is calculated the RES(I) are further modified one at a time, by a factor

$$\frac{\frac{[P * \text{RES}(I)]^2}{\text{VAR}(I)}}{1 + \frac{[P * \text{RES}(I)]^2}{\text{VAR}(I)}}$$

where P is a read-in constant (Card 3) and VAR(I) is the calculated variance for variable I. (When P is not entered a value of 3. is automatically assigned to it.) Basically, when a variance is very large compared to the calculated $(\text{RES})^2$, the factor is very small, and when the variance is small, the factor goes to unity. Modification of the RES(I) starts with the last adjustable one. Once it is adjusted the remaining unmodified RES(I) are recalculated subject to acceptance of the values for the modified ones. Variances for the unmodified RES(I) are recalculated and used for subsequent adjustments.

The modified RES vector is added to the vector of adjustable λ 's, and the values are tested against the imposed upper and lower limits. If a limit is violated the total correction vector RES is scaled down to stay within the most restricting limit. The scaling factor is called CONAB.

A new solution, $q_k^p(t)$ is obtained for the adjusted lambdas. These, together with the $q_k(t)$ of the previous solution and the observed values $q_k^o(t)$ are then used to scale the RES correction vector further to obtain an improvement in the fit of the data. This scaling is based on a linear extrapolation using the relation:

$$\text{CON}_k = \frac{q_k^o(t) - q_k(t)}{q_k^p(t) - q_k(t)} \quad k = 1, \dots, m$$

from which an average scaling factor, CON, is calculated. Because of non-linearities, this adjustment is repeated until the new sum of squares improves by less than $(1-\text{CONMIN})$ of its previous value--or after three tries in any one iteration. The value of CONMIN is read in on Card 3.

If the sum of squares becomes worse, the RES vector is cut down by a factor of ten, and the procedure is repeated.

The best sum of squares obtained during the various adjustment stages is recovered as the final solution of the iteration. A single iteration involves the calculation of partials and the subsequent adjustment of the correction vector.

FINAL RESULTS

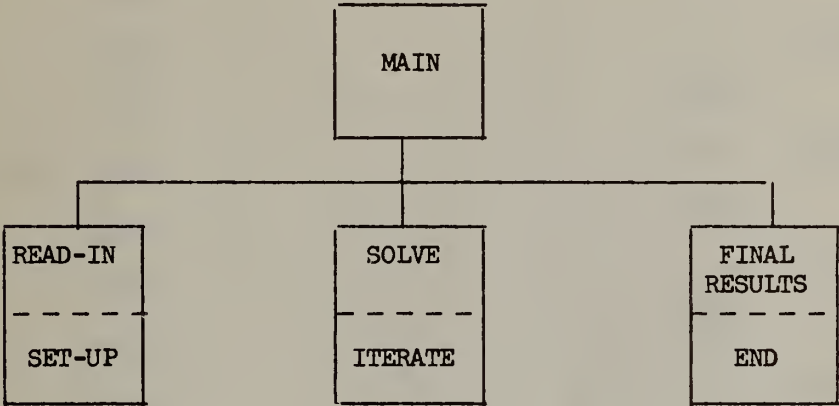
A problem terminates its iterations when the maximum number specified (Card 2) is reached or when fractional improvements in the sum of squares is less than $(1-E)$. The value of E is entered on Card 3. The best solution is retrieved for the final results.

SECTION VIII

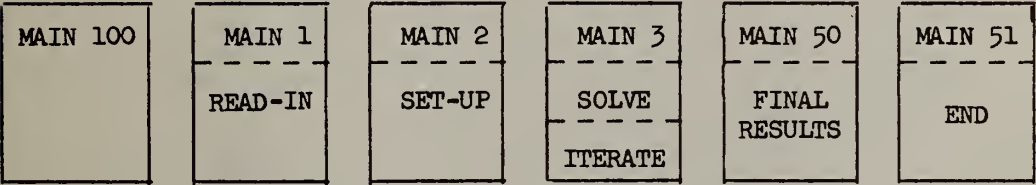
PROGRAM ORGANIZATION

The control of the various computational stages of SAAM is governed by a single main program in an overlay version (FORTRAN IV) and by a series of main programs in a chained version (FORTRAN II). Schematically the two versions may be described as follows:

OVERLAY



CHAIN



Multiple links, each governed by MP3 and containing selected solution routines may be set up for the CHAIN. Dummy routines are used as needed to minimize core requirements.

MAIN PROGRAM (for overlay)

A single main program governs the program flow.

MAIN PROGRAMS (for CHAINS)MAIN 100

MP 0	43
------	----

MAIN 1

MP 1	51
------	----

MAIN 2

MP 2	52
------	----

MAIN 3

MP 3	58
------	----

MAIN 50

MP 50	80
-------	----

MAIN 51

MP 51	89
-------	----

READ-IN

READ0	1
READ1	2
READ2	3
READ3	4
READ4	5
READ5	6
READ6	7
RESRV1	8
READ8	9
DEPCAL	11
K Ø UNTJ	12
PRINT1	13
DECIDE	17
ØRDER	18
TEST	19
READ7	32
HALF1	53
MATNV	64
CLKRD	72
PRINT5	73
YINV	78
READMX	103
ADDMAT	135

SET-UP

JJCALC	10	
DEPEND	20	
MATINV	24	
SETUP	27	
SIZE	42	
SIZPRT	110	(FORTRAN IV version)
MATDIV	44	
SETUP7	47	
HALF2	54	
SETUP5	68	
SETP14	71	
CLKRD	72	
PRINT5	73	
SETP16	76	
YINV	78	
SETP3	97	
SETP11	98	
READMX	103	
SETP17	105	
SETP15	115	
ZGDA1	116	
ZGDA3	118	
SETP18	119	
SETP19	120	
SETP20	121	
WCALC	129	

SOLVE

All solution blocks (of programs) contain the following

JJCALC	10
PRINT2	14
DEPEND	20
STEP	21
DEQSOL	22
SCCALC	23
MATINV	24
SSDET	25
WTSUB	26
STDSS	28
SUB1	29
QCSUM	40
MATDIV	44
HALF3	67
CLKRD	72
PRINT5	73
YINV	78
PRINT7	83
SETSTP	92
PRINT8	94
PARTC	95

and one or more of the following SOLV routines:

SOLV1	46	}
STEP	21	
SETSTP	92	
SOLV2	56	
SOLV3	57	
SOLV5	62	
SOLV6	48	
SOLV7	45	
SOLV8	77	
SOLV9	39	
SOLV10	104	
SOLV11	99	
SOLV12	108	
SOLV13	109	
SOLV14	112	
SOLV15	114	}
ZGDA2	117	
ZGDA3	118	
SOLV16	141	
SOLV17	93	
SOLV18	147	}
GAUS	148	
SOME	150	
SOME1	151	
ERF	149	
SOLV19	161	
SOLV99	70	
QSCALC	152	

ITERATE

PRINT3	15
PRINT4	16
PRTIAL	30
AMX	31
DEVAMX	33
RESDET	34
ADDRES	35
CHNGA	36
CONDET	37
TRMNAT	38
PRINT6	74
HALF5	81
HALF6	82
NEQS	134

FINAL RESULTS

JJCALC	10	
PRINT2	14	
DEPEND	20	
MATINV	24	
CØRCØ	41	
SIZE	42	
SIZPRT	110	(FORTRAN IV version)
MATDIV	44	
HALF7	49	
CLKRD	72	
PRINT5	73	
YINV	78	
PRINT7	83	
PARTC	95	
PUNCH	133	
PUNCH1	136	

END

DEPEND	20
MATINV	24
MATDIV	44
SPCL	55
SPCL1	59
SPCL3	60
PL Ø TT	61
PL Ø T	63
SPCL4	66
SPCL2	69
CLKRD	72
PRINT5	73
YINV	78
PL Ø T1	84
PL Ø T2	85
PL Ø T3	86
PL Ø T10	87
WINDUP	96
WNDP11	100
WNDP12	107
WNDP14	122
WNDP15	123
WNDP16	124
WNDP17	125
WNDP18	126
WNDP19	127
WNDP20	128
WCALC	129
PUNCH	133
HALF8	137
INF Ø	138

SECTION IX

COMMENTS AND SUGGESTIONS

COMPUTING TIME

Problem Solution time refers to the total time necessary to run a problem.

Equation Solution time refers to the time required for a single solution of the model equations to yield values corresponding to all T values specified under "data".

The number of equation solutions (E) necessary to solve a problem cannot be predicted precisely but will lie in the range defined by:

$$(1+V)N + 1 \leq E < (6+V)N + 2$$

where V is the number of independently variable lambdas and N is the number of iterations in the solution. For zero iterations (simulation) $E = 1$.

The time for the solution of a problem equals the time for a single equation solution times the number of equation solutions involved.

The time for a single equation solution depends on the model employed.

a) Analytic solution models. The time for these solutions is usually short and depends mainly on the complexity of the equations and on the number of data points.

b) Numerical solutions. This applies mainly to the solution of differential equations. The time for a single equation solution is approximately proportional to the product

$$LM \times TM \times L$$

where: LM = maximum value of λ_{jj}

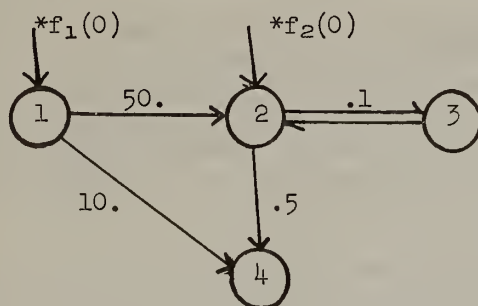
TM = highest T value for data

L = number of lambdas in problem

(For an IBM 7094 a proportionality constant 1.6×10^{-3} will yield the time in seconds.)

T-interrupts may sometimes be employed to reduce computing time in the numerical solution of differential equations. It requires the reduction in the values of the largest λ_{jj} in the model, and can only be done if after such a change the solution remains effectively unaltered.

Consider the following as an example:



The equation solution time of this model is governed by the largest λ_{jj} which is $\lambda_{11} = 50. + 10. = 60.$ However, it is obvious that compartment 1 is essentially depleted after .1 units of time. Thus, a T-interrupt change at $T = .1$, setting $\lambda_{21} = \lambda_{41} = 0$ would not appreciably alter the solution and establish a new λ_{jj} maximum, namely, $\lambda_{22} = .1 + .5 = .6.$ From this time on the solution would proceed about 100 times faster.

CONVERGENCE, UNIQUENESS AND CONSISTENCY

To judge whether a solution has converged and, if so, whether it is consistent and unique, the following measures and hints are useful.

a) Sums of squares (SS) for each "compartment" and total SS (including statistical information) are printed at the end of each iteration. It is necessary for convergence that the improvement in SS for the last iteration be small (a few percent or less compared to previous iteration). This in itself, however, is not sufficient to guarantee convergence.

b) In each iteration a set of corrections is calculated for the independently variable parameters. These corrections are then adjusted by a factor to optimize the fit of the data. The ratio between the actual corrections used and the original corrections calculated is defined CONAB and its value is printed out. CONAB values close to unity at the end of an iteration suggest proper convergence. CONAB values much less than unity suggest that the model may be ill-conditioned, or be non-unique and that convergence to a least squares fit may be very slow.

c) The magnitude of the correction calculated in the beginning of an iteration becomes small compared to the value of the parameter in the neighborhood of a least squares fit.

d) Estimated Standard Deviations are printed out with the final results. These are determined at the beginning of the last iteration. They approximate the "true" estimated standard deviations only if the problem is near a least squares solution at the beginning of the last iteration. Standard deviations which are large compared to parameter

values could mean non-uniqueness of the solution and slow convergence.

e) If the actual fit as inspected by eye seems "good", in that the scatter seems random, and if SS is comparable to a "reference" SS, the solution obtained is near a least squares solution; it may, however, still be non-unique.

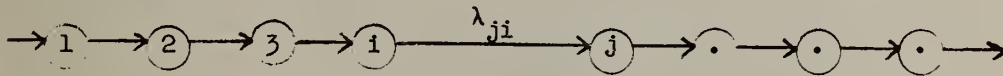
f) If the fit contains systematic deviations but otherwise satisfies all other least squares criteria the solution is inconsistent. The estimated standard deviations for such a solution may be meaningless.

Time-dependent (or T-dependent) λ_{ij}

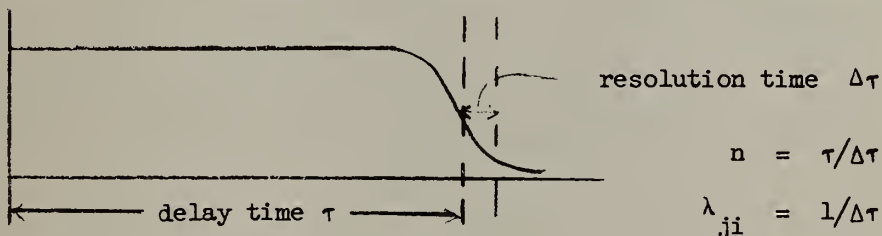
It is possible to solve differential equations (or equivalent models) with time dependent λ_{ij} , provided the function that defines the time dependence can be simulated in SAAM as a component f_k by the use of differential equations. A separate compartmental model is set up to generate the desired function in one of its compartments, say f_k ; the time dependent λ_{ij} is then set equal to f_k through the "f-dependence".

Delays

Frequently it is desired to introduce a delay within a process. For example, iron incorporated in a red cell is not released until the cell "dies". Red cells have a life span of about 120 days and, thus, the iron does not reappear for a time interval which depends on the age of the cell when the iron was incorporated. A 'delay' component is not available in the program. It may, however, be simulated by a number of compartments in series:



If a delay τ is desired, n compartments, each with an average turn-over time τ/n ($\lambda_{ji} = n/\tau$) may be set up in series. All the λ 's may be set equal to each other by dependence relations. The larger the number of compartments n , the closer the series of compartments approach a true time delay. In a rough way, the number of compartments in the chain approximates the ratio of the delay time to the resolution time of the data:

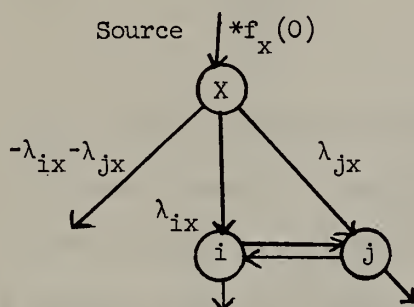


SIMULATION

One can obtain solutions for a model in the absence of any data by entering "dummy" data. Such "data" need have entries only under **COMPONENT** and **T** - leaving everything else on the "data" format blank. The program will assign unit weight for each entry, set the number of iterations to 0 and proceed with a single solution. The calculated values will correspond to the entered "data".

VARIABLE INITIAL CONDITIONS

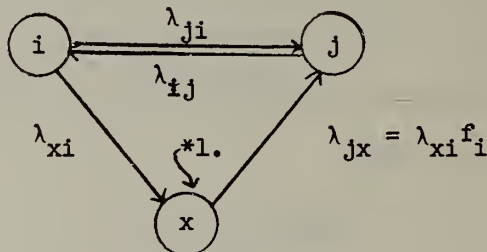
There are no provisions in the program for dealing with variable initial conditions directly. Indirectly, however, this can be accomplished with a "T-interrupt" by introducing "initial conditions" over a finite--but very short--interval of time (instead of instantaneously). A source "feeds" initial conditions into the desired compartments through connecting λ_{ij} which can be made variable. The "feed" period, is terminated by setting the connecting λ_{ij} to zero at the "T-interrupt". The following is an example



Compartment X is the source (a function generator that is constant) for the "feed" and λ_{ix} and λ_{jx} are the "feed" parameters. If the initial condition in compartment X is $f_x(0)$ and λ_{ix} and λ_{jx} are "ON" for a short interval of time τ , the "initial conditions" in compartments i and j respectively will be $\lambda_{ix} f_x(0) \tau$ and $\lambda_{jx} f_x(0) \tau$. It is important that τ be small compared to the reciprocal rate constants in the model.

PARALLEL PATHWAYS

Sometimes one desires to introduce 2 or more parallel pathways between 2 compartments, (for example, the simultaneous presence of passive diffusion and active transport). The program does not permit duplicate parameter designations. This can be accomplished, however, indirectly as follows:



The extra pathway from compartment i to j ($\lambda'_{ji} = \lambda_{xi}$) is diverted to compartment x--a compartment introduced specially for this purpose. This ensures that the right amount of material leaves compartment i. To ensure that the right amount of material reaches j a λ_{jx} is introduced, and through the use of dependence and "f-dependence" is set equal to $\lambda_{xi} f_i$. In addition, the initial condition $f_x(0) = 1$ is introduced into compartment x. It will be observed that this scheme maintains f_x constant: $f_x(t) = 1$, so that $\lambda_{jx} f_i f_x = \lambda_{xi} f_i$.

Comp x can serve simultaneously for a number of extra pathways between various compartments. In fact, by the use of proper dependence relations it can also serve as a source of constant inputs to other compartments.

Additional pathways from comp i to j require independent bypass compartments.

ZEROETH ORDER KINETICS

Frequently the rate of flow from one compartment to another is constant and independent of the amount of material in the compartment. One way to accomplish this is to set the corresponding λ_{ij} proportional to f_j^{-1} --a special case of the f-dependence feature:

$$\lambda_{ij}' f_j = \frac{\lambda_{ij}}{f_j} \cdot f_j = \lambda_{ij}$$

SECTION X

SAMPLE PROBLEMS

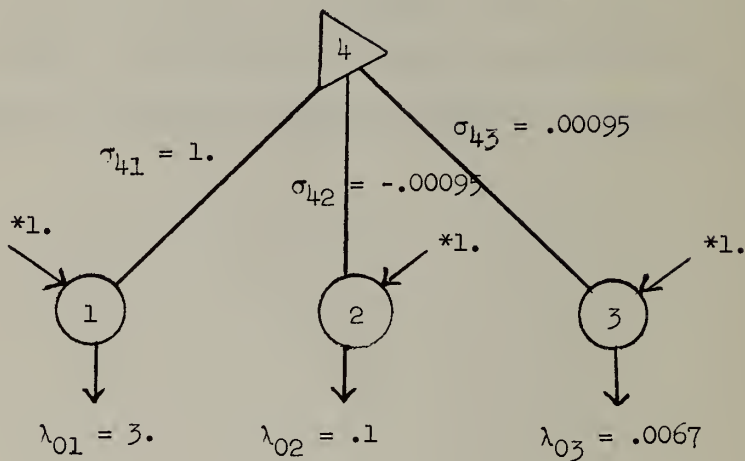
The following are examples of various problems run on SAAM. Features of problems and the SAAM program are presented, usually in an intermixed way. A listing of the data deck required for each example is also given. The first and last 3 rows listed on top and bottom of the data deck are given for the lining up and recognition of columns. These cards are not part of a data deck.

The first card of each data deck contains the problem identification which consists of three initials followed by a number (MAN 002.01). The integer part of the number was chosen to correspond to the model code for the problem so that the reader may readily recognize the type of of problem.

Sum of Exponentials--Simulate

$$q = e^{-3t} - .00095 e^{-.1t} + .00095 e^{-.0067t}$$

Schematic:



$$f_1 = e^{-3t}$$

$$f_2 = e^{-.1t}$$

$$f_3 = e^{-.0067t}$$

$$q_4 = \sigma_{41}f_1 + \sigma_{42}f_2 + \sigma_{43}f_3 = e^{-3t} - .00095 e^{-.1t} + .00095 e^{-.0067t}$$

1 2 3 4 5 6 7 8

12345678901234567890123456789012345678901234567890123456789012345678901234567890

2 saam23 nan002.01 example-sum of exponentials jul 1966

4

.01

.98

.98

3

1

4

4. .5
4. 1.0
4. 1.5
4. 3.0
4. 6.
4. 8.
4. 10.
4. 12.
4. 14.
4. 16.
4. 18.
4. 20.
4. 30.
4. 50.

26

1 1.
2 1.
3 1.

26

26

1 3.
2 .1
3 .0067

26

4 1 1.
4 2 -.00095
4 3 .00095

26

26

26

1

2

3

4

5

6

12345678901234567890123456789012345678901234567890123456789012345678901234567890

1 2 3 4 5 6 7 8

X-3.01

PROBLEM DECK

SAAM23 MAN002.01 EXAMPLE-SUM OF EXPONENTIALS JUL 1966

STARTING TIME= 604.35000

	-0.0000	-0					
	-0.00000	-0.00000	.01000	.98000			.98000
***				-0	-0	-0	-0
4.00000	.5000000	-.0000000		-.0000000	*		-.0000000
4.00000	1.0000000	-.0000000		-.0000000	*		-.0000000
4.00000	1.5000000	-.0000000		-.0000000	*		-.0000000
4.00000	3.0000000	-.0000000		-.0000000	*		-.0000000
4.00000	6.0000000	-.0000000		-.0000000	*		-.0000000
4.00000	8.0000000	-.0000000		-.0000000	*		-.0000000
4.00000	10.0000000	-.0000000		-.0000000	*		-.0000000
4.00000	12.0000000	-.0000000		-.0000000	*		-.0000000
4.00000	14.0000001	-.0000000		-.0000000	*		-.0000000
4.00000	16.0000000	-.0000000		-.0000000	*		-.0000000
4.00000	18.0000000	-.0000000		-.0000000	*		-.0000000
4.00000	20.0000000	-.0000000		-.0000000	*		-.0000000
4.00000	30.0000000	-.0000000		-.0000000	*		-.0000000
4.00000	50.0000000	-.0000000		-.0000000	*		-.0000000
20.00000	-.0000000	-.0000000		-.0000000	*		-.0000000
***ALL WEIGHTS=1.**2*							
1	1.0000000			-.0000000			-.0000000
2	1.0000000			-.0000000			-.0000000
3	1.0000000			-.0000000			-.0000000
26	-.0000000			-.0000000			-.0000000
26 -0	-.0000000	-.0000000		-.0000000	-0		-.0000000
-0 1	3.0000000	-.0000000		-.0000000	-0		-.0000000
-0 2	.1000000	-.0000000		-.0000000	-0		-.0000000
-0 3	.0067000	-.0000000		-.0000000	-0		-.0000000
26 -0	-.0000000	-.0000000		-.0000000	-0		-.0000000
4 1	1.0000000	-.0000000		-.0000000	-0		-.0000000
4 2	-.0009500	-.0000000		-.0000000	-0		-.0000000
4 3	.0009500	-.0000000		-.0000000	-0		-.0000000
26 -0	-.0000000	-.0000000		-.0000000	-0		-.0000000
26 -0	-0 -0	-.0000000		-.0000000			
26 -0	-.0000000	-.0000000		-.0000000			

REORGANIZED PROBLEM INFORMATION

N.I.M.
MATHEMATICAL RESEARCH BRANCH
PROGRAM SAHM 23
NUMBER OF COMPONENTS IS 4
NUMBER OF DATA POINTS IS 14

DATA

C	T	GC	W
4	.500000+00	-.000000	.100000+01
4	.100000+01	-.000000	.100000+01
4	.150000+01	-.000000	.100000+01
4	.300000+01	-.000000	.100000+01
4	.600000+01	-.000000	.100000+01
4	.800000+01	-.000000	.100000+01
4	.100000+02	-.000000	.100000+01
4	.120000+02	-.000000	.100000+01
4	.140000+02	-.000000	.100000+01
4	.160000+02	-.000000	.100000+01
4	.180000+02	-.000000	.100000+01
4	.200000+02	-.000000	.100000+01
4	.300000+02	-.000000	.100000+01
4	.500000+02	-.000000	.100000+01

INITIAL CONDITIONS

I	F(I,0)	JUDY(I)	V(I)	H(I)	GP AT .0000	GP AT .0000	GP AT .0000	GP AT .0000
1	.100000+01	1	-.000000	-.000000	.000000	.000000	.000000	.000000
2	.100000+01	1	-.000000	-.000000	.000000	.000000	.000000	.000000
3	.100000+01	1	-.000000	-.000000	.000000	.000000	.000000	.000000
4	.000000	2	.000000	.000000	.000000	.000000	.000000	.000000

PARAMETERS

ADJUSTABLE	DEPENDENT	FIXED	
INITIAL ESTIMATE	MIN	MAX	VALUE

LAMBDA (0, 1) =	.3000000+01
LAMBDA (0, 2) =	.1000000+00
LAMBDA (0, 3) =	.6700000-02
SIGMA (4, 1) =	.1000000+01
SIGMA (4, 2) =	-.9500000-03
SIGMA (4, 3) =	.9500000-03

NO DEPENDENCE RELATIONSHIPS

NO INDEPENDENT STATISTICAL CONSTRAINTS

***NO ADJUSTABLE LAMBDA'S. ITERATIONS SET TO ZERO. ***19*

SOLUTION

MODEL CODE= 2

ESTIMATE OF SIG FROM REAP-IN DATA= .0000000

LAMBDA (1, 1) = -.3000000+01
LAMBDA (2, 2) = -.1000000+00
LAMBDA (3, 3) = -.6700000-02

PARAMETER VALUES

ADJUSTABLE PARAMETERS

DEPENDENT PARAMETERS

FIXED PARAMETERS

U	C	T	GC/K	K	GC	GO	GO-GC	GC/GO
1	4	.500000+00	.223173-00	.100000+01	.223173-00	-.000000	-.223173-00	.0000
2	4	.100000+01	.496711-01	.100000+01	.496711-01	-.000000	-.496711-01	.0000
3	4	.150000+01	.112318-01	.100000+01	.112318-01	-.000000	-.112318-01	.0000
4	4	.300000+01	.350728-03	.100000+01	.350728-03	-.000000	-.350728-03	.0000
5	4	.600000+01	.391212-03	.100000+01	.391212-03	-.000000	-.391212-03	.0000
6	4	.800000+01	.473558-03	.100000+01	.473558-03	-.000000	-.473558-03	.0000
7	4	.100000+02	.538950-03	.100000+01	.538950-03	-.000000	-.538950-03	.0000
8	4	.120000+02	.590475-03	.100000+01	.590475-03	-.000000	-.590475-03	.0000
9	4	.140000+02	.630674-03	.100000+01	.630674-03	-.000000	-.630674-03	.0000
10	4	.160000+02	.661627-03	.100000+01	.661627-03	-.000000	-.661627-03	.0000
11	4	.180000+02	.685035-03	.100000+01	.685035-03	-.000000	-.685035-03	.0000
12	4	.200000+02	.702292-03	.100000+01	.702292-03	-.000000	-.702292-03	.0000
13	4	.300000+02	.729719-03	.100000+01	.729719-03	-.000000	-.729719-03	.0000
14	4	.500000+02	.673170-03	.100000+01	.673170-03	-.000000	-.673170-03	.0000

SOL. SAVED AFTER 0 ITERATIONS IS .52423531-01

COMP 4= .52423531-01

SIG AFTER 0 ITERATIONS IS .57445379-02

***NO ADJUSTABLE PARAMETERS**07*

SOLUTION TYPE= .000000

Sum of Exponentials--Fit

Fit a sum of three exponentials

$$q = A_1 e^{-\alpha_1 t} + A_2 e^{-\alpha_2 t} + A_3 e^{-\alpha_3 t}$$

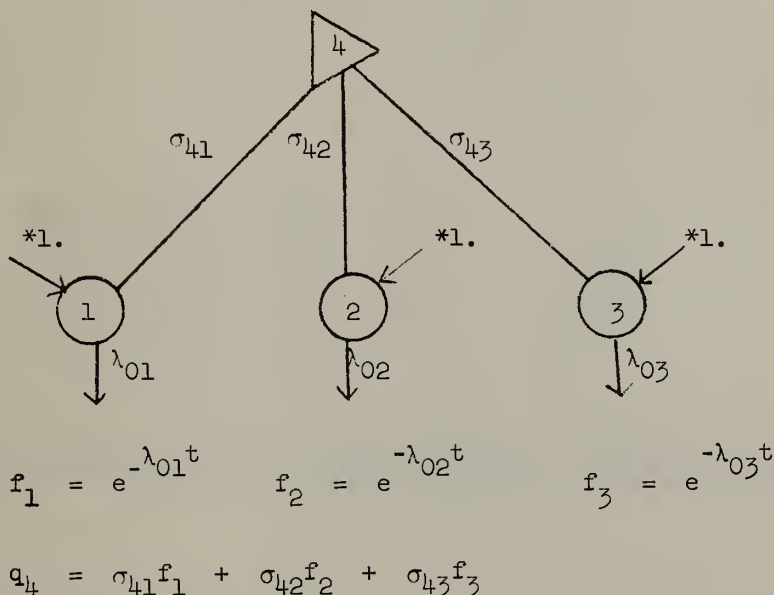
to the following data, given initial estimates $\alpha_1 = 1$, $\alpha_2 = .1$, $\alpha_3 = .0007$

Data:

t	.5	1.	1.5	3.	6.	8.	.10	.12
observed	.22	.049	.0112	.00033	.00036	.00043	.00049	.00054

	14.	16.	18.	20.	30.	50.
	.000575	.00061	.00063	.00065	.000675	.00061

Schematic:



Note: The upper and lower limits on σ_{41} , σ_{42} , σ_{43} and λ_{01} , λ_{02} , λ_{03} are somewhat arbitrary.

The data deck is shown on the following page.

$$\Delta T_{\text{m}}(141\text{K}) = 1004.45530$$
[illegible]

NEURON-4721 FUGLE™ INFECTION

NATIONAL RESTRICTION STATUS
 PROGRAM NAME 25
 NUMBER OF COMPONENTS IS 4
 NUMBER OF DATA POINTS IS 14

٥٨١ع.

	1	2	3
4	.500000+00	.220000-00	.637262-05
4	.000000+01	.490000-01	.128461-03
4	.150000+01	.112000-01	.245602-02
4	.200000+01	.300000-03	.203220+01
4	.000000+01	.300000-03	.237990+01
4	.000000+01	.430000-03	.106612+01
4	.100000+02	.490000-03	.128461+01
4	.120000+02	.590000-03	.105773+01
4	.240000+02	.600000-03	.432000+00
4	.100000+02	.010000-03	.026703-00
4	.100000+02	.030000-03	.777110-00
4	.000000+02	.650000-03	.730023-00
4	.300000+02	.075000-03	.676949-00
4	.500000+02	.010000-03	.020903-00

THE CONSTITUTION

I	F(I,0)	JULY(I)	V(I)	U(I)	GP AT .0000	GP AT .0000	GP AT .0000	GP AT .0000
1	.10000+01	1	-.00000	-.00000	.000000	.000000	.000000	.000000
2	.10000+01	1	-.00000	-.00000	.000000	.000000	.000000	.000000
3	.10000+01	1	-.00000	-.00000	.000000	.000000	.000000	.000000
4	.000000	2	.00000	.00000	.000000	.000000	.000000	.000000

PARAMETERS

ADJUSTABLE
INITIAL ESTIMATE

414

MAX

DEPENDENT

FIXED

VALUE

LAMBDA (0, 1)=	.30000000+01	-.6000	.5000+01
LAMBDA (0, 2)=	.10000000+00	-.0000	.5000+01
LAMBDA (0, 3)=	.67000000-02	-.0000	.5000+01
SIGMA (4, 1)=	-.00000000	-.1000+03	.1000+03
SIGMA (4, 2)=	-.00000000	-.1000+03	.1000+03
SIGMA (4, 3)=	-.00000000	-.1000+03	.1000+03

NO DEPENDENCE RELATIONSHIPS

NO INDEPENDENT STATISTICAL CONSTRAINTS

SOLUTION

MODEL CODE= 2
ESTIMATE OF SIG FROM READ-IN DATA= .7710871-09

X-50K

LAMBDA(1, 1) = -.3000000+01
LAMBDA(2, 2) = -.1000000+00
LAMBDA(3, 3) = -.6700000-02

PARAMETER VALUES

ADJUSTABLE PARAMETERS

SIGMA (1, 1) = .9988869-00
SIGMA (1, 2) = -.6720618-03
SIGMA (1, 3) = .6708863-03
LAMBDA(1, 1) = .3000000+01
LAMBDA(1, 2) = .1000000+00
LAMBDA(1, 3) = .6700000-02

DEPENDENT PARAMETERS

FIXED PARAMETERS

L	C	T	CC/K	K	CC	CO	CC-CC	CC/CO
1	4	.500000+00	.226089-00	.100000+01	.220089-00	.720000-00	-.688942-03	1.0031
2	4	.100000+01	.493098-01	.100000+01	.493098-01	.190000-01	-.309783-03	1.0063
3	4	.150000+01	.110771-01	.100000+01	.110971-01	.112000-01	.102650-03	.9908
4	4	.300000+01	.329027-03	.100000+01	.329027-03	.130000-03	.432934-06	.9987
5	4	.100000+01	.356000-03	.100000+01	.356000-03	.130000-03	.200004-05	.9944
6	4	.100000+01	.433000-03	.100000+01	.433000-03	.130000-03	-.360453-05	1.0084
7	4	.100000+01	.493098-03	.100000+01	.493098-03	.140000-03	-.268630-05	1.0074
8	4	.120000+02	.546359-03	.100000+01	.540959-03	.140000-03	-.958971-06	1.0018
9	4	.140000+02	.577074-03	.100000+01	.577074-03	.175000-03	-.287440-05	1.0050
10	4	.160000+02	.606302-03	.100000+01	.606302-03	.110000-03	.369825-05	.9939
11	4	.180000+02	.627003-03	.100000+01	.627803-03	.130000-03	.219600-05	.9965
12	4	.200000+02	.643058-03	.100000+01	.673058-03	.150000-03	.634175-05	.9902
13	4	.300000+02	.661911-03	.100000+01	.660911-03	.175000-03	.609887-05	.9910
14	4	.500000+02	.617111-03	.100000+01	.617111-03	.110000-03	-.711081-05	1.0117

SUM SQUARES AFTER 0 ITERATIONS IS .2103910E-09
COMP 4E .2103911-09
SIG AFTER 0 ITERATIONS IS .1917640E-10

SOLUTION TIME = .00000

ITERATION NUMBER 1

DETERMINANT OF A-MATRIX = 1+ANIL00 -.1090770E2

1	ORIG.RES	MOD.RES	ORIG. CR	LITTLE CR	COND.NO.	LITTLE A(1,1)	MOD.VAR.(1,1)
1	-.59123-02	-.401360-02	-.221574-00	-.479932-05	.10000+01	.44963-03	.82378-05
2	-.19154-02	-.180319-02	-.128484-00	.15421+05	.10101+01	.20834-02	.40071-00
3	.10170-02	.10721-02	.62767-07	.91394-05	.20973+01	.05796-02	.64253-07

CORRECTIONS FOR ADJUSTABLE LAMBDA

RES(1) = -.4310704E-02

RES(2) = -.900380E-02

RES(3) = .157200E-02

COND = .1000000+01

PARAMETER VALUES

ADJUSTABLE PARAMETERS

SIGMA (1, 1) = .9932385-00
SIGMA (1, 2) = -.932534E-03
SIGMA (1, 3) = .6407055-03
LAMBDA(1, 1) = .2499104+01
LAMBDA(1, 2) = .5130814-01
LAMBDA(1, 3) = .6272834-02

DEPENDENT PARAMETERS

FIXED PARAMETERS

SUM SQUARES AFTER 1 ITERATIONS IS .10373593-09
COMP 4E .1037359-09
SIG AFTER 1 ITERATIONS IS .9430530E-11
SUM SQUARES AFTER 1 ITERATIONS IS .10374646-09
COMP 4E .1037465-09
SIG AFTER 1 ITERATIONS IS .94314960-11
COND AFTER 1 TIMES IN THE 1TH ITERATION = .1093213+01
SUM SQUARES AFTER 1 ITERATIONS IS .10359254-09
COMP 4E .1035925-09
SIG AFTER 1 ITERATIONS IS .94175035-11

TOTAL RES FOR ITERATION 1

RES(1) = -.5280612E-02

RES(2) = -.9430460E-02

RES(3) = .1719440E-02

ITERATION TIME = .00000

ITERATION NUMBER 2

DETERMINANT OF A-MATRIX = 1+ANIL00 -.105040+02

1	ORIG.RES	MOD.RES	ORIG. CR	LITTLE CR	COND.NO.	LITTLE A(1,1)	MOD.VAR.(1,1)
1	-.51317-03	-.43960-05	.21332-09	.47051-06	.10000+01	.45338-03	.79005-07
2	.40164-03	.51640-03	.52718-00	.18362-05	.10904+01	.29632-02	.11777-00
3	.60650-04	.45517-05	.27440-07	.20405-06	.30405+01	.47793-02	.34264-00

CORRECTIONS FOR ADJUSTABLE LAMBDA

RES(1) = -.4396610-05

RES(2) = .5104794-03

RES(3) = .4551670-05

X-5.03 CONAB = .1000000+01

PARAMETER VALUES

ADJUSTABLE PARAMETERS

SIGMA (4, 1)= .9828683-00
SIGMA (4, 2)= -.9386879-03
SIGMA (4, 3)= .9460415-03
LAMBDA(U, 1)= .2994709+01
LAMBDA(U, 2)= .9108002-01
LAMBDA(U, 3)= .8423994-02

DEPENDENT PARAMETERS

FIXED PARAMETERS

SUM SQUARES AFTER 2 ITERATIONS IS .10019912-09
COMP 4= .1001991-09
SIG AFTER 2 ITERATIONS IS .91090112-11
CONAB AFTER 1 TRIES IN THE 2TH ITERATION = .1234991+01

SUM SQUARES AFTER 2 ITERATIONS IS .10007064-09
COMP 4= .1000708-09
SIG AFTER 2 ITERATIONS IS .90973494-11

TOTAL RES FOR ITERATION 2
RES(1) = -.54240227-05
RES(2) = .63764700-03
RES(3) = .56212302-05

ITERATION TIME= .01606

ITERATION NUMBER 3 -----

DETERMINANT OF A-MATRIX= 1*ANTILOG -.165008+02

INFORMATION CONNECTED WITH CALCULATION AND MODIFICATION OF RES

I	ORIG.RES	MOD.RES	ORIG. CR	LITTLE CR	COND.NO.	LITTLE A(I,1)	MOD.VAR.(I,1)
1	-.52058-03	-.44448-04	-.12114-09	-.26729-06	.10000+01	.45322-03	.35410-06
2	-.21995-03	.16660-06	-.24455-11	.11535-06	.10906+01	.25674-02	.86581-09
3	.51772-04	.30141-05	.16155-08	.24997-06	.30226+01	.48283-02	.25243-08

CONNECTIONS FOR ADJUSTABLE LAMBDA

RES(1) = -.4444810-04
RES(2) = .1666009-06
RES(3) = .3014106-05

CONAB = .1000000+01

PARAMETER VALUES

ADJUSTABLE PARAMETERS

SIGMA (4, 1)= .9828674-00

DEPENDENT PARAMETERS

FIXED PARAMETERS

SIGMA (4, 2)= -.9387069-03
SIGMA (4, 3)= .9456869-03
LAMBDA(U, 1)= .2994663+01
LAMBDA(U, 2)= .9120155-01
LAMBDA(U, 3)= .8428078-02

SUM SQUARES AFTER 3 ITERATIONS IS .10003379-09
COMP 4= .1000538-09
SIG AFTER 3 ITERATIONS IS .90957990-11
CONAB AFTER 1 TRIES IN THE 3TH ITERATION = .5074069+01

SUM SQUARES AFTER 3 ITERATIONS IS .10002329-09
COMP 4= .1000233-09
SIG AFTER 3 ITERATIONS IS .90930264-11

TOTAL RES FOR ITERATION 3
RES(1) = -.22551417-03
RES(2) = .84470958-06
RES(3) = .15293830-04

ITERATION TIME= .00000

PARAMETER VALUES

ADJUSTABLE PARAMETERS

SIGMA (4 1) = .9027010-00
 SIGMA (4 2) = -.9392094-00
 SIGMA (4 3) = .9404720-00
 LAMBDA (0 1) = .2994460+01
 LAMBDA (0 2) = .9120220-01
 LAMBDA (0 3) = .2440330-02

DEPENDENT PARAMETERS

FIXED PARAMETERS

	U	C	T	CC/P	K	UC	GO	GO=GO	GC/GO	F.S.D.
1	4	.500000+00	.219921-00	.100000+01	.249921-00	.220000-00	.791345-04	.9996	.3689-02	
2	4	.100000+01	.492773-01	.100000+01	.492773-01	.490000-01	-.277293-03	1.0057	.3923-03	
3	4	.150000+01	.111121-01	.100000+01	.111220-01	.112000-01	.774203-04	.9931	.3650-02	
4	4	.300000+01	.331300-03	.100000+01	.331300-03	.330000-03	-.130020-05	1.0039	.2771-02	
5	4	.600000+01	.335957-03	.100000+01	.335957-03	.330000-03	.404307-05	.9888	.2039-02	
6	4	.800000+01	.431490-03	.100000+01	.431490-03	.430000-03	-.148992-05	1.0035	.2022-02	
7	4	.100000+02	.492164-03	.100000+01	.492164-03	.490000-03	-.218365-05	1.0045	.1828-02	
8	4	.120000+02	.540037-03	.100000+01	.540037-03	.540000-03	-.537344-06	1.0010	.1442-02	
9	4	.140000+02	.576046-03	.100000+01	.576046-03	.575000-03	-.364568-05	1.0063	.1123-02	
10	4	.160000+02	.616530-03	.100000+01	.616530-03	.610000-03	.174655-05	.9971	.1123-02	
11	4	.180000+02	.660614-03	.100000+01	.660614-03	.650000-03	-.813947-06	1.0013	.1426-02	
12	4	.200000+02	.697528-03	.100000+01	.697528-03	.690000-03	.246248-05	.9962	.1824-02	
13	4	.300000+02	.672536-03	.100000+01	.672536-03	.675000-03	.146357-05	.9976	.2980-02	
14	4	.300000+02	.610517-03	.100000+01	.610517-03	.610000-03	-.519300-06	1.0009	.4838-02	

SUM SQUARES AFTER 3 ITERATIONS IS .10002329-09

COEFF 42 .1000233-09

SIG AFTER 3 ITERATIONS IS .90930264-14

STANDARD DEVIATIONS

FRACTIONAL DEVIATIONS

ADJUSTABLE PARAMETERS

SIGMA (4 1) = .9027010-00+00 = .0023529-02 .8105-02
 SIGMA (4 2) = -.9392094-00+00 = .2647350-04 .2712-01
 SIGMA (4 3) = .9404720-00+00 = .2970700-04 .3140-01
 LAMBDA (0 1) = .2994460+01+00 = .7575060-02 .2530-02
 LAMBDA (0 2) = .9120220-01+00 = .3405120-02 .3734-01
 LAMBDA (0 3) = .2440330-02+00 = .0240604-03 .7401-01

CORRELATION MATRIX

	1	2	3	4	5	6
R01	1.00	-.40	.29	.00	.00	.00
R02	-.40	1.00	-.94	.00	.00	.00
R03	.29	-.94	1.00	.00	.00	.00
R04	.00	.00	.00	1.00	-.15	.09
R05	.00	.00	.00	-.15	1.00	-.91
R06	.00	.00	.00	.09	-.91	1.00

COMPONENT 4 OF PROBLEM NO. -0000 SHAN23 MAR002.02 EXAMPLE-SUM OF EXPONENTIALS JUL 1966

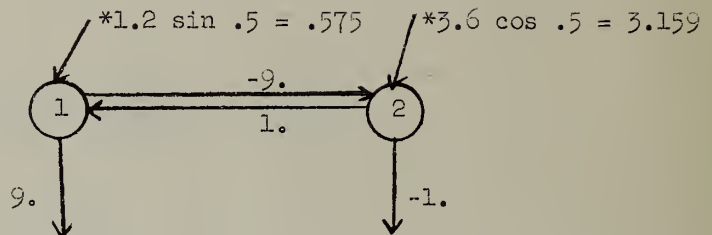
RUNNING TIME = .0168 (MINUTES - UNICAL 1108)

Sine function - Simulate (1.02)

Simulate the sine function

$$q = 1.2 \sin(3t + .5)$$

Schematic



$$\frac{df_1}{dt} = f_2$$

$$f_1(0) = A \sin a = 1.2 \sin .5$$

$$\frac{df_2}{dt} = \omega^2 f_1 = -9 f_1$$

$$f_2(0) = A \omega \cos a = 3.6 \cos .5$$

$$q = f_1 = 1.2 \sin(3t + .5)$$

1	2	3	4	5	6	7	8
1234567890123456789012345678901234567890123456789012345678901234567890							

2 saan23 man 1.02 simulate sine function

01.02 2 .01 .98 .98

3 options

1. .0

1. .01

1. .02

1. .03

1. .04

1. .05

200. .05

50.

2.

200. .01

5.

200. .05

50.

26

1 .575

2 3.159

26

26

1 2 1.

2 1 -9.

0 1 9.

0 2 -1.

26

26

26

26

1234567890123456789012345678901234567890123456789012345678901234567890							
1	2	3	4	5	6	7	8

SAAMES PLAN 1.02 SIMULATE SINE FUNCTION.

STARTING FILE=1064.45000

```

      1.020      2      -0
      -.00000      -.00000      .01000      .36000      -0      -.98000
**3**
      1.00000      .0000000      -.0000000      -.0000000 *      -0      -0
      1.00000      .0100000      -.0000000      -.0000000 *      -.0000000
      1.00000      .0200000      -.0000000      -.0000000 *      -.0000000
      1.00000      .0300000      -.0000000      -.0000000 *      -.0000000
      1.00000      .0400000      -.0000000      -.0000000 *      -.0000000
      1.00000      .0500000      -.0000000      -.0000000 *      -.0000000
      2.00.00000      .0500000      -.0000000      50.0000000 *      -.0000000
      2.00.00000      -.0000000      -.0000000      -.0000000 *      -.0000000
      2.00.00000      .0100000      -.0000000      -.0000000 *      -.0000000
      2.00.00000      .0500000      -.0000000      50.0000000 *      -.0000000
      2.00.00000      -.0000000      -.0000000      -.0000000 *      -.0000000

**ALL *LIBRIS=1.**2*
      1      .3750000      -.0000000      -.0000000
      2      3.1590000      -.0000000      -.0000000
      20      -.0000000      -.0000000      -.0000000
      20 -0      -.0000000      -.0000000      -0      -.0000000
      1 2      1.0000000      -.0000000      -.0000000      -0      -.0000000
      2 1      -.0000000      -.0000000      -.0000000      -0      -.0000000
      0 1      9.0000000      -.0000000      -.0000000      -0      -.0000000
      0 2      -1.0000000      -.0000000      -.0000000      -0      -.0000000
      20 -0      -.0000000      -.0000000      -.0000000      -0      -.0000000
      20 -0      -.0000000      -.0000000      -.0000000      -0      -.0000000
      20 -0      -0      -0      -0      -0      -0
      20 -0      -.0000000      -.0000000      -.0000000

```

REORGANIZED PROBLEM INFORMATION

11-1-11
 MATHEMATICAL RESEARCH BRANCH
 PROGRAM SAAM 23
 NUMBER OF COMPONENTS IS 2
 NUMBER OF DATA POINTS IS 112

DATA

```

      C      1      GC      W
      1      .000000      -.000000      .100000+01
      1      .100000-01      .000000      .100000+01
      1      .200000-01      -.000000      .100000+01
      1      .300000-01      -.000000      .100000+01
      1      .400000-01      -.000000      .100000+01
      1      .500000-01      -.000000      .100000+01
      1      .100000+00      .000000      .100000+01
      1      .150000-00      .000000      .100000+01
      1      .200000-00      .000000      .100000+01
      1      .250000-00      .000000      .100000+01
      1      .300000-00      .000000      .100000+01
      1      .350000-00      .000000      .100000+01
      1      .400000-00      .000000      .100000+01
      1      .450000-00      .000000      .100000+01
      1      .500000-00      .000000      .100000+01
      1      .550000-00      .000000      .100000+01
      1      .600000-00      .000000      .100000+01
      1      .650000-00      .000000      .100000+01
      1      .700000-00      .000000      .100000+01
      1      .750000-00      .000000      .100000+01
      1      .800000-00      .000000      .100000+01
      1      .850000-00      .000000      .100000+01
      1      .900000-00      .000000      .100000+01
      1      .950000-00      .000000      .100000+01
      1      .100000+01      .000000      .100000+01
      1      .105000+01      .000000      .100000+01
      1      .110000+01      .000000      .100000+01
      1      .115000+01      .000000      .100000+01
      1      .120000+01      .000000      .100000+01
      1      .125000+01      .000000      .100000+01
      1      .130000+01      .000000      .100000+01
      1      .135000+01      .000000      .100000+01
      1      .140000+01      .000000      .100000+01
      1      .145000+01      .000000      .100000+01
      1      .150000+01      .000000      .100000+01
      1      .155000+01      .000000      .100000+01
      1      .160000+01      .000000      .100000+01
      1      .165000+01      .000000      .100000+01
      1      .170000+01      .000000      .100000+01
      1      .175000+01      .000000      .100000+01
      1      .180000+01      .000000      .100000+01
      1      .185000+01      .000000      .100000+01
      1      .190000+01      .000000      .100000+01
      1      .195000+01      .000000      .100000+01
      1      .200000+01      .000000      .100000+01
      1      .205000+01      .000000      .100000+01

```

- . I 1997+01

.59848+01

	.000000	1		*	+
*	.100000-001	1		*	+
	.200000-001	1		*	+
*	.300000-001	1		*	+
	.400000-001	1		*	+
*	.500000-001	1		*	+
	.100000+001	1		*	+
	.100000-001	1		*	+
	.200000-001	1	*		+
	.250000-001	1	*		+
	.300000-001	1	*		+
	.350000-001	1	*		+
	.400000-001	1	*		+
	.450000-001	1	*		+
	.500000-001	1	*		+
	.550000-001	1	*		+
	.600000-001	1	*		+
	.650000-001	1	*		+
	.700000-001	1	*		+
	.750000-001	1	*		+
	.800000-001	1	*		+
	.850000-001	1	++		
	.900000-001	1	++		
	.950000-001	1	++		
	.100000+001	1	+	*	
	.105000+001	1	+	*	
	.110000+001	1	+	*	
	.115000+001	1	+	*	

.120000+011	I			
I		+		*
.125000+011	I		+	*
I				
.130000+011	I	+		*
I				
.135000+011	I		+	*
I				
.140000+011	I	+		*
I				
.145000+011	I		+	*
I				
.150000+011	I	+		*
I				
.155000+011	I		+	*
I				
.160000+011	I		+	*
I				
.165000+011	I	+		*
I				
.170000+011	I		+	*
I				
.175000+011	I		+	*
I				
.180000+011	I		+	*
I				
.185000+011	I		+	*
I				
.190000+011	I			**
I				
.195000+011	I			**
I				
.200000+011	I		+	+
I				
.205000+011	I		+	+
I				
.210000+011	I		*	+
I				
.215000+011	I		*	+
I				
.220000+011	I		*	+
I				
.225000+011	I		*	+
I				
.230000+011	I		*	+
I				
.235000+011	I		*	+
I				
.240000+011	I		*	+
I				
.245000+011	I		*	+
I				
.250000+011	I		*	

Differential Equations - Simulate:

$$q_1 = 10 f_1$$

$$q_2 = f_2$$

$$q_7 = f_1 + .5 f_2$$

where f_1 and f_2 are the solutions of

$$\frac{df_1}{dt} = -3 f_1 + 2 f_2 + 1.2 \sin(3t + .5)$$

$$\frac{df_2}{dt} = 1 f_1 - 2.5 f_2 + 0.5 e^{-2t}$$

$$f_1(0) = 0$$

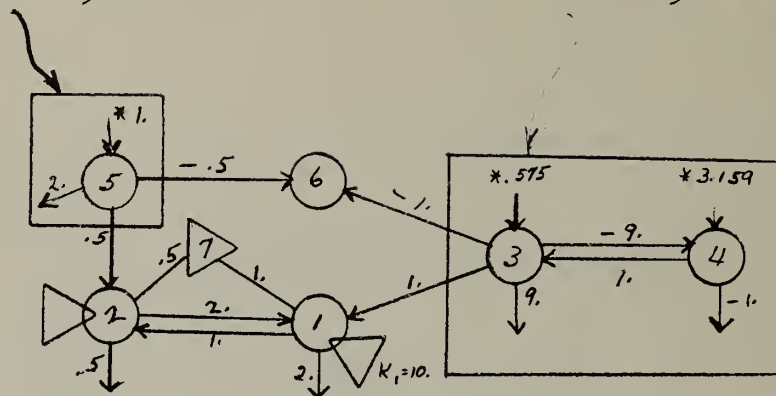
$$f_2(0) = 0$$

Simulate above for 3 units of time, then cut off input function to f_1 $[1.2 \sin(3t + .5)]$. Continue solution for 3 more units of time and cut off input function to f_2 $[.5 e^{-2t}]$, and observe solution for 3 more units of time after that. Obtain values for q_1 and q_2 in intervals of .1 units of time over entire simulation period and values for q_7 in intervals of .1 units of time over last period only.

Schematic:

$$G_1(t) = f_5(t) = e^{-2t}$$

$$G_2(t) = f_3(t) = 1.2 \sin(3t + .5)$$



Component 6 is a "dummy" introduced for convenience only as a "sink" for the compensating pathways.

$G_1(t)$ and $G_2(t)$ are function generators.

1 2 3 4 5 6 7 8
 1234567890123456789012345678901234567890123456789012345678901234567890

2 saan23 man 1.03 simulate diff equat w/sin and exp inputs
 01.03 7

.01 .98 .98

4
 1. 0.
 200. .1 30.
 2. 30.
 200. .1 30.
 126. 1.
 1. 30.
 200. .1 30.
 2. 30.
 200. .1 30.
 126. 1. 1.
 1. 3.
 200. .1 30.
 2. 3.
 200. .1 30.
 7. 3.
 200. .1 30.

26
 3 .575
 4 3.159
 5 1.

26
 1 10.

26
 1 2 2.
 2 1 1.
 0 1 2.
 0 2 .5
 3 4 1.
 4 3 -9.
 0 3 9.
 0 4 -1.
 1 3 1.
 6 3 -1.
 0 5 2.
 2 5 .5
 6 5 -.5

1234567890123456789012345678901234567890123456789012345678901234567890
 1 2 3 4 5 6 7 8

(continued on next page)

(continued)

1	2	3	4	5	6	7	8
1234567890123456789012345678901234567890123456789012345678901234567890							

7	1	1.
7	2	.5
26		
26		
26		
26		
26		
1	3	
2	5	
26		
26		

1234567890123456789012345678901234567890123456789012345678901234567890							
1	2	3	4	5	6	7	8

Note: cards with "200." entry under COMP are "data generation control cards".

In this problem they generate 30 points in increments of 0.1 units of t , starting with value of t just preceding the control card (or last t value generated by previous data generation control card).

X-9.01

PROBLEM DECK

SAAN25 MAR 1.03 SIMULATE DIFF EQUAT W/SIN AND EXP INPUTS

STARTING TIME= 604.36666

1.030	7	-0					
-0.00000		-0.00000	.01000	.98000	-0	-0	.98000
***					-0	-0	-0
1.00000	.0000000	-0.000000		-0.000000	*		-0.000000
200.00000	.1000000	-0.000000		30.000000	*		-0.000000
2.00000	-0.000000	-0.000000		-0.000000	*		-0.000000
200.00000	.1000000	-0.000000		30.000000	*		-0.000000
120.00000	-0.000000	1.000000		-0.000000	*		-0.000000
1.00000	-0.000000	-0.000000		-0.000000	*		-0.000000
200.00000	.1000000	-0.000000		30.000000	*		-0.000000
2.00000	-0.000000	-0.000000		-0.000000	*		-0.000000
200.00000	.1000000	-0.000000		30.000000	*		-0.000000
120.00000	1.000000	1.000000		-0.000000	*		-0.000000
1.00000	3.000000	-0.000000		-0.000000	*		-0.000000
200.00000	.1000000	-0.000000		30.000000	*		-0.000000
2.00000	3.000000	-0.000000		-0.000000	*		-0.000000
200.00000	.1000000	-0.000000		30.000000	*		-0.000000
7.00000	3.000000	-0.000000		-0.000000	*		-0.000000
200.00000	.1000000	-0.000000		30.000000	*		-0.000000
20.00000	-0.000000	-0.000000		-0.000000	*		-0.000000

***ALL WEIGHTS=1.**2*

3		.5750000		-0.000000		-0.000000
4		3.1590000		-0.000000		-0.000000
5		1.000000		-0.000000		-0.000000
26		-0.000000		-0.000000		-0.000000
1	-0	10.000000	-0.000000	-0.000000	-0	-0.000000
26	-0	-0.000000	-0.000000	-0.000000	-0	-0.000000
1	2	2.000000	-0.000000	-0.000000	-0	-0.000000
2	1	1.000000	-0.000000	-0.000000	-0	-0.000000
0	1	2.000000	-0.000000	-0.000000	-0	-0.000000
0	2	.5000000	-0.000000	-0.000000	-0	-0.000000
3	4	1.000000	-0.000000	-0.000000	-0	-0.000000
4	3	-9.000000	-0.000000	-0.000000	-0	-0.000000
0	3	9.000000	-0.000000	-0.000000	-0	-0.000000
0	4	-1.000000	-0.000000	-0.000000	-0	-0.000000
1	3	1.000000	-0.000000	-0.000000	-0	-0.000000
0	3	-1.000000	-0.000000	-0.000000	-0	-0.000000
0	5	2.000000	-0.000000	-0.000000	-0	-0.000000
2	5	.5000000	-0.000000	-0.000000	-0	-0.000000
0	5	-0.500000	-0.000000	-0.000000	-0	-0.000000
26	-0	-0.000000	-0.000000	-0.000000	-0	-0.000000
7	1	1.000000	-0.000000	-0.000000	-0	-0.000000
7	2	.5000000	-0.000000	-0.000000	-0	-0.000000
26	-0	-0.000000	-0.000000	-0.000000	-0	-0.000000
26	-0	-0	-0.000000	-0.000000	-0	-0.000000
26	-0	-0.000000	-0.000000	-0.000000	-0	-0.000000
26	-0	-0.000000	-0.000000	-0.000000	-0	-0.000000
1	3	-0.000000	-0.000000	-0	-0	-0
2	5	-0.000000	-0.000000	-0	-0	-0

26	-0	-0.000000	-0.000000	-0	-0
26	-0	-0.000000	-0.000000	-0	-0

X-9.04

INITIAL CONDITIONS

	F(1,0)	JUST(1)	V(1)	(1)	UP AT	-1.000+01	UP AT	-1.000+01	UP AT	-1.000	UP AT	-1.000
1	.00000	1	.00000	.00000	.00000		.00000		.00000		.00000	
2	.00000	1	.00000	.00000	.00000		.00000		.00000		.00000	
3	.375 0+00	1	-.00000	-.00000	.00000		.00000		.00000		.00000	
4	-.3125+01	1	-.00000	-.00000	.00000		.00000		.00000		.00000	
5	.1000+01	1	-.00000	-.00000	.00000		.00000		.00000		.00000	
6	.08000	1	.00000	.00000	.00000		.00000		.00000		.00000	
7	.06000	2	.00000	.00000	.00000		.00000		.00000		.00000	

F(1) NODES TO AT 1-INTERMPT 1
F(1) NODES TO AT 1-INTERMPT 2

PARAMETERS

	ADJUSTABLE INITIAL ESTIMATE	MIN	MAX	DEPENDENT	FIXED	VALUE
					LAMBDA (1, 0)=	.100000+02
					LAMBDA (1, 2)=	.200000+01
					LAMBDA (2, 1)=	.100000+01
					LAMBDA (0, 1)=	.200000+01
					LAMBDA (0, 2)=	.500000-00
					LAMBDA (3, 4)=	.100000+01
					LAMBDA (4, 3)=	-.900000+01
					LAMBDA (0, 3)=	.900000+01
					LAMBDA (0, 4)=	-.100000+01
					LAMBDA (1, 3)=	-.100000+01
					LAMBDA (6, 3)=	-.100000+01
					LAMBDA (0, 5)=	.200000+01
					LAMBDA (2, 5)=	.500000-00
					LAMBDA (6, 5)=	-.500000-00
					SIGMA (7, 1)=	.100000+01
					SIGMA (7, 2)=	.500000-00

END OF DATA ENDED AT 1-INTERMPT 1
END OF (1, 0)= -.00000000 END OF (1, 2)= -.00000000
END OF (2, 1)= -.00000000 END OF (0, 1)= -.00000000

RELATIONSHIPS

RELATIONSHIPS SIGNIFICANT COEFFICIENTS

*** ADJUSTABLE COEFFICIENTS SET TO ZERO ***194

SOLUTION

NODES 1
END OF DATA ENDED AT 1-INTERMPT 1

END OF (1, 1)= -.70 0000+01
END OF (0, 1)= -.200000+01
END OF (2, 1)= .000000
END OF (4, 1)= .000000

END OF (5, 1)= -.200000+01
END OF (6, 1)= .000000

PARAMETER VALUES

ADJUSTABLE PARAMETERS

DEPENDENT PARAMETERS

FIXED PARAMETERS

LAMBDA (1, 0)= .100000+02
SIGMA (7, 1)= .100000+01
LAMBDA (1, 2)= .200000+01
LAMBDA (2, 1)= .100000+01
LAMBDA (0, 1)= .200000+01
LAMBDA (0, 2)= .500000-00
LAMBDA (3, 4)= .100000+01
LAMBDA (4, 3)= -.900000+01
LAMBDA (0, 3)= .900000+01
LAMBDA (0, 4)= -.100000+01
LAMBDA (1, 3)= -.100000+01
LAMBDA (6, 3)= -.100000+01
LAMBDA (0, 5)= .200000+01
LAMBDA (2, 5)= .500000-00
LAMBDA (6, 5)= -.500000-00

INITIAL POINTS

	C	T	W	A	W	0	00-00	W/00
1	.10000	.00000	.10000+02	.00000	.00000	-.00000	-.00000	.0000
2	.10000+00	.17184+01	.10000+02	.17184+00	.00000	-.67353+00	.0000	.0000
3	.00000+00	.14407+01	.10000+02	.14407+00	.00000	-.14407+01	.0000	.0000
7	.00000+00	.21095+00	.10000+02	.21095+00	.00000	-.22095+01	.0000	.0000
9	.00000+00	.20601+00	.10000+02	.20601+01	.00000	-.20601+01	.0000	.0000
11	.00000+00	.30402+00	.10000+02	.30402+01	.00000	-.33402+01	.0000	.0000
13	.00000+00	.30575+00	.10000+02	.30575+01	.00000	-.35775+01	.0000	.0000
15	.00000+00	.30575+00	.10000+02	.30575+01	.00000	-.35775+01	.0000	.0000
17	.00000+00	.30575+00	.10000+02	.30575+01	.00000	-.35775+01	.0000	.0000
19	.00000+00	.20575+00	.10000+02	.20575+01	.00000	-.20575+01	.0000	.0000
21	.00000+00	.21707+00	.10000+02	.21707+01	.00000	-.21707+01	.0000	.0000
23	.00000+00	.10606+00	.10000+02	.10606+01	.00000	-.10606+01	.0000	.0000
25	.00000+00	.09617+00	.10000+02	.09617+00	.00000	-.09617+00	.0000	.0000
27	.00000+00	.00000+00	.10000+02	.00000+00	.00000	.00000+00	.0000	.0000
29	.00000+00	-.11371+00	.10000+02	-.11371+01	.00000	.11371+01	.0000	.0000
31	.00000+00	-.17509+00	.10000+02	-.17509+01	.00000	.17509+01	.0000	.0000
33	.00000+00	-.21709+00	.10000+02	-.21709+01	.00000	.21709+01	.0000	.0000
35	.00000+00	-.23553+00	.10000+02	-.23553+01	.00000	.23553+01	.0000	.0000
37	.00000+00	-.22843+00	.10000+02	-.22843+01	.00000	.22843+01	.0000	.0000
39	.00000+00	-.19724+00	.10000+02	-.19724+01	.00000	.19724+01	.0000	.0000
41	.00000+00	-.14509+00	.10000+02	-.14509+01	.00000	.14509+01	.0000	.0000
43	.00000+00	-.70092+00	.10000+02	-.70092+01	.00000	.70092+01	.0000	.0000
45	.00000+00	-.06524+00	.10000+02	-.06524+01	.00000	.06524+01	.0000	.0000
47	.00000+00	-.01069+00	.10000+02	-.01069+01	.00000	.01069+01	.0000	.0000
49	.00000+00	-.11631+00	.10000+02	-.11631+01	.00000	.11631+01	.0000	.0000
51	.00000+00	-.21900+00	.10000+02	-.21900+01	.00000	.21900+01	.0000	.0000
53	.00000+00	-.26508+00	.10000+02	-.26508+01	.00000	.26508+01	.0000	.0000
55	.00000+00	-.26508+00	.10000+02	-.26508+01	.00000	.26508+01	.0000	.0000
57	.00000+00	-.26764+00	.10000+02	-.26764+01	.00000	.26764+01	.0000	.0000
59	.00000+00	-.26239+00	.10000+02	-.26239+01	.00000	.26239+01	.0000	.0000
61	.00000+00	-.21481+00	.10000+02	-.21481+01	.00000	.21481+01	.0000	.0000

FIXED PA. AIRTEKS

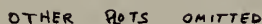
		T	Δ	C	Δ	0C-3L	0C/00
06	4	-7.0000e-01	-7.1414e-01	1.0000e+02	-2.4461e+01	-7.0000e-01	-7.2141e+01
07	4	-1.0000e+00	-1.1200e+00	1.0000e+02	-1.1266e+01	-7.0000e-01	-1.1726e+01
07	4	-2.0000e+00	-2.1414e+00	1.0000e+02	-1.1406e+01	-7.0000e-01	-1.1414e+01
07	4	-3.0000e+00	-3.1729e+00	1.0000e+02	-1.1729e+01	-7.0000e-01	-1.1729e+01
07	4	-4.0000e+00	-4.2043e+00	1.0000e+02	-1.2043e+01	-7.0000e-01	-1.2043e+01
73	4	-1.0000e+00	-1.1414e-01	1.0000e+02	-3.4413e-01	-7.0000e-01	-7.3413e-01
75	4	-6.0000e-01	-7.1423e-01	1.0000e+02	-7.1232e-01	-6.0000e-01	-7.1232e-01
77	4	-7.0000e-01	-8.1264e-01	1.0000e+02	-8.1264e-01	-6.0000e-01	-8.1264e-01
77	4	-8.0000e-01	-9.1244e-01	1.0000e+02	-9.1244e-01	-6.0000e-01	-9.1244e-01
81	4	-9.0000e-01	-1.0271e-01	1.0000e+02	-2.0271e-01	-7.0000e-01	-1.0271e-01
83	4	-1.0000e+01	-1.2794e+01	1.0000e+02	-1.2794e+01	-6.0000e-01	-1.2794e+01
83	4	-1.1000e+01	-1.3465e+01	1.0000e+02	-1.3465e+01	-7.0000e-01	-1.3465e+01
84	4	-1.2000e+01	-1.4077e+01	1.0000e+02	-1.4077e+01	-6.0000e-01	-1.4077e+01
84	4	-1.3000e+01	-1.4642e+01	1.0000e+02	-1.4642e+01	-7.0000e-01	-1.4642e+01
85	4	-1.4000e+01	-1.5194e+01	1.0000e+02	-1.5194e+01	-6.0000e-01	-1.5194e+01
85	4	-1.5000e+01	-1.5735e+01	1.0000e+02	-1.5735e+01	-7.0000e-01	-1.5735e+01
86	4	-1.6000e+01	-1.6265e+01	1.0000e+02	-1.6265e+01	-6.0000e-01	-1.6265e+01
86	4	-1.7000e+01	-1.6784e+01	1.0000e+02	-1.6784e+01	-7.0000e-01	-1.6784e+01
87	4	-1.8000e+01	-1.7291e+01	1.0000e+02	-1.7291e+01	-6.0000e-01	-1.7291e+01
87	4	-1.9000e+01	-1.7786e+01	1.0000e+02	-1.7786e+01	-7.0000e-01	-1.7786e+01
88	4	-2.0000e+01	-1.8269e+01	1.0000e+02	-1.8269e+01	-6.0000e-01	-1.8269e+01
88	4	-2.1000e+01	-1.8740e+01	1.0000e+02	-1.8740e+01	-7.0000e-01	-1.8740e+01
89	4	-2.2000e+01	-1.9199e+01	1.0000e+02	-1.9199e+01	-6.0000e-01	-1.9199e+01
89	4	-2.3000e+01	-1.9646e+01	1.0000e+02	-1.9646e+01	-7.0000e-01	-1.9646e+01
90	4	-2.4000e+01	-2.0081e+01	1.0000e+02	-2.0081e+01	-6.0000e-01	-2.0081e+01
90	4	-2.5000e+01	-2.0504e+01	1.0000e+02	-2.0504e+01	-7.0000e-01	-2.0504e+01
91	4	-2.6000e+01	-2.0915e+01	1.0000e+02	-2.0915e+01	-6.0000e-01	-2.0915e+01
91	4	-2.7000e+01	-2.1314e+01	1.0000e+02	-2.1314e+01	-7.0000e-01	-2.1314e+01
92	4	-2.8000e+01	-2.1701e+01	1.0000e+02	-2.1701e+01	-6.0000e-01	-2.1701e+01
92	4	-2.9000e+01	-2.2075e+01	1.0000e+02	-2.2075e+01	-7.0000e-01	-2.2075e+01
93	4	-3.0000e+01	-2.2437e+01	1.0000e+02	-2.2437e+01	-6.0000e-01	-2.2437e+01
93	4	-3.1000e+01	-2.2787e+01	1.0000e+02	-2.2787e+01	-7.0000e-01	-2.2787e+01
94	4	-3.2000e+01	-2.3125e+01	1.0000e+02	-2.3125e+01	-6.0000e-01	-2.3125e+01
94	4	-3.3000e+01	-2.3451e+01	1.0000e+02	-2.3451e+01	-7.0000e-01	-2.3451e+01
95	4	-3.4000e+01	-2.3765e+01	1.0000e+02	-2.3765e+01	-6.0000e-01	-2.3765e+01
95	4	-3.5000e+01	-2.4067e+01	1.0000e+02	-2.4067e+01	-7.0000e-01	-2.4067e+01
96	4	-3.6000e+01	-2.4357e+01	1.0000e+02	-2.4357e+01	-6.0000e-01	-2.4357e

[illegible]

I=ITERATION

125	1	.300000+01	.279733-02	.100000+02	.279733-01	-.000000	-.279733-01	.0000
126	1	.310000+01	.245246-02	.100000+02	.245246-01	.000000	-.245246-01	.0000
131	1	.320000+01	.215043-02	.100000+02	.215043-01	.000000	-.215043-01	.0000
134	1	.330000+01	.186800-02	.100000+02	.186800-01	.000000	-.186800-01	.0000
137	1	.340000+01	.158557-02	.100000+02	.158557-01	.000000	-.158557-01	.0000
140	1	.350000+01	.145015-02	.100000+02	.145015-01	.000000	-.145015-01	.0000
143	1	.360000+01	.127160-02	.100000+02	.127160-01	.000000	-.127160-01	.0000
146	1	.370000+01	.111504-02	.100000+02	.111504-01	.000000	-.111504-01	.0000
149	1	.380000+01	.977751-03	.100000+02	.977751-02	.000000	-.977751-02	.0000
152	1	.390000+01	.857368-03	.100000+02	.857368-02	.000000	-.857368-02	.0000
155	1	.400000+01	.751307-03	.100000+02	.751307-02	.000000	-.751307-02	.0000
158	1	.410000+01	.659276-03	.100000+02	.659276-02	.000000	-.659276-02	.0000
161	1	.420000+01	.578077-03	.100000+02	.578077-02	.000000	-.578077-02	.0000
164	1	.430000+01	.506902-03	.100000+02	.506902-02	.000000	-.506902-02	.0000
167	1	.440000+01	.444493-03	.100000+02	.444493-02	.000000	-.444493-02	.0000
170	1	.450000+01	.389767-03	.100000+02	.389767-02	.000000	-.389767-02	.0000
173	1	.460000+01	.341770-03	.100000+02	.341770-02	.000000	-.341770-02	.0000
176	1	.470000+01	.299698-03	.100000+02	.299698-02	.000000	-.299698-02	.0000
179	1	.480000+01	.262799-03	.100000+02	.262799-02	.000000	-.262799-02	.0000
182	1	.490000+01	.230443-03	.100000+02	.230443-02	.000000	-.230443-02	.0000
185	1	.500000+01	.202071-03	.100000+02	.202071-02	.000000	-.202071-02	.0000
188	1	.510000+01	.177192-03	.100000+02	.177192-02	.000000	-.177192-02	.0000
191	1	.520000+01	.155370-03	.100000+02	.155370-02	.000000	-.155370-02	.0000
194	1	.530000+01	.136246-03	.100000+02	.136246-02	.000000	-.136246-02	.0000
197	1	.540000+01	.119471-03	.100000+02	.119471-02	.000000	-.119471-02	.0000
200	1	.550000+01	.104762-03	.100000+02	.104762-02	.000000	-.104762-02	.0000
203	1	.560000+01	.918637-04	.100000+02	.918637-03	.000000	-.918637-03	.0000
206	1	.570000+01	.805534-04	.100000+02	.805534-03	.000000	-.805534-03	.0000
209	1	.580000+01	.706357-04	.100000+02	.706357-03	.000000	-.706357-03	.0000
212	1	.590000+01	.619390-04	.100000+02	.619390-03	.000000	-.619390-03	.0000
215	1	.600000+01	.543130-04	.100000+02	.543130-03	.000000	-.543130-03	.0000
218	1	.610000+01	.475798-04	.100000+01	.475798-02	-.000000	-.235798-02	.0000
221	1	.620000+01	.420677-04	.100000+01	.420677-02	.000000	-.206770-02	.0000
224	1	.630000+01	.371315-04	.100000+01	.371315-02	.000000	-.181315-02	.0000
227	1	.640000+01	.326992-04	.100000+01	.326992-02	.000000	-.159992-02	.0000
230	1	.650000+01	.289418-04	.100000+01	.289418-02	.000000	-.139418-02	.0000
233	1	.660000+01	.256254-04	.100000+01	.256254-02	.000000	-.122254-02	.0000
236	1	.670000+01	.227020-04	.100000+01	.227020-02	.000000	-.107202-02	.0000
239	1	.680000+01	.200436-03	.100000+01	.200436-03	.000000	-.040036-03	.0000
242	1	.690000+01	.176430-03	.100000+01	.176430-03	.000000	-.028130-03	.0000
245	1	.700000+01	.154813-03	.100000+01	.154813-03	.000000	-.025267-03	.0000
248	1	.710000+01	.135307-03	.100000+01	.135307-03	.000000	-.022159-03	.0000
251	1	.720000+01	.117607-03	.100000+01	.117607-03	.000000	-.194230-03	.0000
254	1	.730000+01	.101960-03	.100000+01	.101960-03	.000000	-.170350-03	.0000
257	1	.740000+01	.870555-03	.100000+01	.870555-03	.000000	-.149380-03	.0000
260	1	.750000+01	.755755-03	.100000+01	.755755-03	.000000	-.130993-03	.0000
263	1	.760000+01	.657557-03	.100000+01	.657557-03	.000000	-.114868-03	.0000
266	1	.770000+01	.572557-03	.100000+01	.572557-03	.000000	-.100723-03	.0000
269	1	.780000+01	.500000-03	.100000+01	.500000-03	.000000	-.883218-04	.0000
272	1	.790000+01	.438557-03	.100000+01	.438557-03	.000000		
275	1	.800000+01	.387557-03	.100000+01	.387557-03	.000000		
278	1	.810000+01	.346557-03	.100000+01	.346557-03	.000000		
281	1	.820000+01	.315557-03	.100000+01	.315557-03	.000000		
284	1	.830000+01	.294557-03	.100000+01	.294557-03	.000000		
287	1	.840000+01	.273557-03	.100000+01	.273557-03	.000000		
290	1	.850000+01	.252557-03	.100000+01	.252557-03	.000000		
293	1	.860000+01	.231557-03	.100000+01	.231557-03	.000000		
296	1	.870000+01	.210557-03	.100000+01	.210557-03	.000000		
299	1	.880000+01	.189557-03	.100000+01	.189557-03	.000000		
302	1	.890000+01	.168557-03	.100000+01	.168557-03	.000000		
305	1	.900000+01	.147557-03	.100000+01	.147557-03	.000000		
308	1	.910000+01	.126557-03	.100000+01	.126557-03	.000000		
311	1	.920000+01	.105557-03	.100000+01	.105557-03	.000000		
314	1	.930000+01	.845557-03	.100000+01	.845557-03	.000000		
317	1	.940000+01	.635557-03	.100000+01	.635557-03	.000000		
320	1	.950000+01	.425557-03	.100000+01	.425557-03	.000000		
323	1	.960000+01	.215557-03	.100000+01	.215557-03	.000000		
326	1	.970000+01	.005557-03	.100000+01	.005557-03	.000000		
329	1	.980000+01	-.205557-03	.100000+01	-.205557-03	.000000		
332	1	.990000+01	-.405557-03	.100000+01	-.405557-03	.000000		
335	1	.000000+01	-.605557-03	.100000+01	-.605557-03	.000000		
338	1	.010000+01	-.805557-03	.100000+01	-.805557-03	.000000		
341	1	.020000+01	-.100557-02	.100000+01	-.100557-02	.000000		
344	1	.030000+01	-.300557-02	.100000+01	-.300557-02	.000000		
347	1	.040000+01	-.500557-02	.100000+01	-.500557-02	.000000		
350	1	.050000+01	-.700557-02	.100000+01	-.700557-02	.000000		
353	1	.060000+01	-.900557-02	.100000+01	-.900557-02	.000000		
356	1	.070000+01	-.100557-01	.100000+01	-.100557-01	.000000		
359	1	.080000+01	-.300557-01	.100000+01	-.300557-01	.000000		
362	1	.090000+01	-.500557-01	.100000+01	-.500557-01	.000000		
365	1	.100000+01	-.700557-01	.100000+01	-.700557-01	.000000		
368	1	.110000+01	-.900557-01	.100000+01	-.900557-01	.000000		
371	1	.120000+01	-.100557-00	.100000+01	-.100557-00	.000000		
374	1	.130000+01	-.300557-00	.100000+01	-.300557-00	.000000		
377	1	.140000+01	-.500557-00	.100000+01	-.500557-00	.000000		
380	1	.150000+01	-.700557-00	.100000+01	-.700557-00	.000000		
383	1	.160000+01	-.900557-00	.100000+01	-.900557-00	.000000		
386	1	.170000+01	-.100557-00	.100000+01	-.100557-00	.000000		
389	1	.180000+01	-.300557-00	.100000+01	-.300557-00	.000000		
392	1	.190000+01	-.500557-00	.100000+01	-.500557-00	.000000		
395	1	.200000+01	-.700557-00	.100000+01	-.700557-00	.000000		
398	1	.210000+01	-.900557-00	.100000+01	-.900557-00	.000000		
401	1	.220000+01	-.100557-00	.100000+01	-.100557-00	.000000		
404	1	.230000+01	-.300557-00	.100000+01	-.300557-00	.000000		
407	1	.240000+01	-.500557-00	.100000+01	-.500557-00	.000000		
410	1	.250000+01	-.700557-00	.100000+01	-.700557-00	.000000		
413	1	.260000+01	-.900557-00	.100000+01	-.900557-00	.000000		
416	1	.270000+01	-.100557-00	.100000+01	-.100557-00	.000000		
419	1	.280000+01	-.300557-00	.100000+01	-.300557-00	.000000		
422	1	.290000+01	-.500557-00	.100000+01	-.500557-00	.000000		
425	1	.300000+01	-.700557-00	.100000+01	-.700557-00	.000000		
428	1	.310000+01	-.900557-00	.100000+01	-.900557-00	.000000		
431	1	.320000+01	-.100557-00	.100000+01	-.100557-00	.000000		
434	1	.330000+01	-.300557-00	.100000+01	-.300557-00	.000000		
437	1	.340000+01	-.500557-00	.100000+01	-.500557-00	.000000		
440	1	.350000+01	-.700557-00	.100000+01	-.700557-00	.000000		
443	1	.360000+01	-.900557-00	.100000+01	-.900557-00	.000000		
446	1	.370000+01	-.100557-00	.100000+01	-.100557-00	.000000		
449	1	.380000+01	-.300557-00	.100000+01	-.300557-00	.000000		
452	1	.390000+01	-.500557-00	.100000+01	-.500557-00	.000000		
455	1	.400000+01	-.700557-00	.100000+01	-.700557-00	.000000		
458	1	.410000+01	-.900557-00	.100000+01	-.900557-00	.000000		
461	1	.420000+01	-.100557-00	.100000+01	-.100557-00	.000000		
464	1	.430000+01	-.300557-00	.100000+01	-.300557-00	.000000		
467	1	.440000+01	-.500557-00	.100000+01	-.500557-00	.000000		
470	1	.450000+01	-.700557-00	.100000+01	-.700557-00	.000000		
473	1	.460000+01	-.900557-00	.100000+01	-.900557-00	.000000		
476	1	.470000+01	-.100557-00	.100000+01	-.100557-00	.000000		
479	1	.480000+01	-.300557-00	.100000+01	-.300557-00	.000000		
482	1	.490000+01	-.500557-00	.100000+01	-.500557-00	.000000		
485	1	.500000+01	-.700557-00	.100000+01	-.700557-00	.000000		
488	1	.51000						

UNION OF SOVIET REPUBLICS, 1986, 200-201, 1. 2. 3. 4. 5. 6. 7. 8. 9. 10. 11. 12. 13. 14. 15. 16. 17. 18. 19. 20. 21. 22. 23. 24. 25. 26. 27. 28. 29. 30. 31. 32. 33. 34. 35. 36. 37. 38. 39. 40. 41. 42. 43. 44. 45. 46. 47. 48. 49. 50. 51. 52. 53. 54. 55. 56. 57. 58. 59. 60. 61. 62. 63. 64. 65. 66. 67. 68. 69. 70. 71. 72. 73. 74. 75. 76. 77. 78. 79. 80. 81. 82. 83. 84. 85. 86. 87. 88. 89. 90. 91. 92. 93. 94. 95. 96. 97. 98. 99. 100. 101. 102. 103. 104. 105. 106. 107. 108. 109. 110. 111. 112. 113. 114. 115. 116. 117. 118. 119. 120. 121. 122. 123. 124. 125. 126. 127. 128. 129. 130. 131. 132. 133. 134. 135. 136. 137. 138. 139. 140. 141. 142. 143. 144. 145. 146. 147. 148. 149. 150. 151. 152. 153. 154. 155. 156. 157. 158. 159. 160. 161. 162. 163. 164. 165. 166. 167. 168. 169. 170. 171. 172. 173. 174. 175. 176. 177. 178. 179. 180. 181. 182. 183. 184. 185. 186. 187. 188. 189. 190. 191. 192. 193. 194. 195. 196. 197. 198. 199. 200. 201. 202. 203. 204. 205. 206. 207. 208. 209. 210. 211. 212. 213. 214. 215. 216. 217. 218. 219. 220. 221. 222. 223. 224. 225. 226. 227. 228. 229. 230. 231. 232. 233. 234. 235. 236. 237. 238. 239. 240. 241. 242. 243. 244. 245. 246. 247. 248. 249. 250. 251. 252. 253. 254. 255. 256. 257. 258. 259. 260. 261. 262. 263. 264. 265. 266. 267. 268. 269. 270. 271. 272. 273. 274. 275. 276. 277. 278. 279. 280. 281. 282. 283. 284. 285. 286. 287. 288. 289. 290. 291. 292. 293. 294. 295. 296. 297. 298. 299. 300. 301. 302. 303. 304. 305. 306. 307. 308. 309. 310. 311. 312. 313. 314. 315. 316. 317. 318. 319. 320. 321. 322. 323. 324. 325. 326. 327. 328. 329. 330. 331. 332. 333. 334. 335. 336. 337. 338. 339. 340. 341. 342. 343. 344. 345. 346. 347. 348. 349. 350. 351. 352. 353. 354. 355. 356. 357. 358. 359. 360. 361. 362. 363. 364. 365. 366. 367. 368. 369. 370. 371. 372. 373. 374. 375. 376. 377. 378. 379. 380. 381. 382. 383. 384. 385. 386. 387. 388. 389. 390. 391. 392. 393. 394. 395. 396. 397. 398. 399. 400. 401. 402. 403. 404. 405. 406. 407. 408. 409. 410. 411. 412. 413. 414. 415. 416. 417. 418. 419. 420. 421. 422. 423. 424. 425. 426. 427. 428. 429. 430. 431. 432. 433. 434. 435. 436. 437. 438. 439. 440. 441. 442. 443. 444. 445. 446. 447. 448. 449. 450. 451. 452. 453. 454. 455. 456. 457. 458. 459. 460. 461. 462. 463. 464. 465. 466. 467. 468. 469. 470. 471. 472. 473. 474. 475. 476. 477. 478. 479. 480. 481. 482. 483. 484. 485. 486. 487. 488. 489. 490. 491. 492. 493. 494. 495. 496. 497. 498. 499. 500. 501. 502. 503. 504. 505. 506. 507. 508. 509. 510. 511. 512. 513. 514. 515. 516. 517. 518. 519. 520. 521. 522. 523. 524. 525. 526. 527. 528. 529. 530. 531. 532. 533. 534. 535. 536. 537. 538. 539. 540. 541. 542. 543. 544. 545. 546. 547. 548. 549. 550. 551. 552. 553. 554. 555. 556. 557. 558. 559. 560. 561. 562. 563. 564. 565. 566. 567. 568. 569. 570. 571. 572. 573. 574. 575. 576. 577. 578. 579. 580. 581. 582. 583. 584. 585. 586. 587. 588. 589. 590. 591. 592. 593. 594. 595. 596. 597. 598. 599. 600. 601. 602. 603. 604. 605. 606. 607. 608. 609. 610. 611. 612. 613. 614. 615. 616. 617. 618. 619. 620. 621. 622. 623. 624. 625. 626. 627. 628. 629. 630. 631. 632. 633. 634. 635. 636. 637. 638. 639. 640. 641. 642. 643. 644. 645. 646. 647. 648. 649. 650. 651. 652. 653. 654. 655. 656. 657. 658. 659. 660. 661. 662. 663. 664. 665. 666. 667. 668. 669. 670. 671. 672. 673. 674. 675. 676. 677. 678. 679. 680. 681. 682. 683. 684. 685. 686. 687. 688. 689. 690. 691. 692. 693. 694. 695. 696. 697. 698. 699. 700. 701. 702. 703. 704. 705. 706. 707. 708. 709. 710. 711. 712. 713. 714. 715. 716. 717. 718. 719. 720. 721. 722. 723. 724. 725. 726. 727. 728. 729. 730. 731. 732. 733. 734. 735. 736. 737. 738. 739. 740. 741. 742. 743. 744. 745. 746. 747. 748. 749. 750. 751. 752. 753. 754. 755. 756. 757. 758. 759. 760. 761. 762. 763. 764. 765. 766. 767. 768. 769. 770. 771. 772. 773. 774. 775. 776. 777. 778. 779. 780. 781. 782. 783. 784. 785. 786. 787. 788. 789. 790. 791. 792. 793. 794. 795. 796. 797. 798. 799. 800. 801. 802. 803. 804. 805. 806. 807. 808. 809. 810. 811. 812. 813. 814. 815. 816. 817. 818. 819. 820. 821. 822. 823. 824. 825. 826. 827. 828. 829. 830. 831. 832. 833. 834. 835. 8



RUNNING TIME = .083 (MIN - UNIVAC 1108)

Similarity Transformation - Simulate

Given

$$\lambda = \begin{vmatrix} .95265 & .01450 & .03283 \\ -1. & .4 & .6 \\ .07 & -.3 & .23 \end{vmatrix}$$

$$M = \begin{vmatrix} 1.29571 & 0 & 0 \\ 0 & .2133503 & 0 \\ 0 & 0 & .00732722 \end{vmatrix}$$

Calculate

$$F = \lambda M \lambda^{-1}$$

26

12345678901234567890123456789012345678901234567890123456789012345678901234567890

217.871.42 111.1=1004.56000

0	1	2	3	4	5	6	7	8	9	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z																																																																																																																																																																																																																												
00000000	00000001	00000010	00000011	00000100	00000101	00000110	00000111	00001000	00001001	00001010	00001011	00001100	00001101	00001110	00001111	00010000	00010001	00010010	00010011	00010100	00010101	00010110	00010111	00011000	00011001	00011010	00011011	00011100	00011101	00011110	00011111	00100000	00100001	00100010	00100011	00100100	00100101	00100110	00100111	00101000	00101001	00101010	00101011	00101100	00101101	00101110	00101111	00110000	00110001	00110010	00110011	00110100	00110101	00110110	00110111	00111000	00111001	00111010	00111011	00111100	00111101	00111110	00111111	01000000	01000001	01000010	01000011	01000100	01000101	01000110	01000111	01001000	01001001	01001010	01001011	01001100	01001101	01001110	01001111	01010000	01010001	01010010	01010011	01010100	01010101	01010110	01010111	01011000	01011001	01011010	01011011	01011100	01011101	01011110	01011111	01100000	01100001	01100010	01100011	01100100	01100101	01100110	01100111	01101000	01101001	01101010	01101011	01101100	01101101	01101110	01101111	01110000	01110001	01110010	01110011	01110100	01110101	01110110	01110111	01111000	01111001	01111010	01111011	01111100	01111101	01111110	01111111	10000000	10000001	10000010	10000011	10000100	10000101	10000110	10000111	10001000	10001001	10001010	10001011	10001100	10001101	10001110	10001111	10010000	10010001	10010010	10010011	10010100	10010101	10010110	10010111	10011000	10011001	10011010	10011011	10011100	10011101	10011110	10011111	10100000	10100001	10100010	10100011	10100100	10100101	10100110	10100111	10101000	10101001	10101010	10101011	10101100	10101101	10101110	10101111	10110000	10110001	10110010	10110011	10110100	10110101	10110110	10110111	10111000	10111001	10111010	10111011	10111100	10111101	10111110	10111111	11000000	11000001	11000010	11000011	11000100	11000101	11000110	11000111	11001000	11001001	11001010	11001011	11001100	11001101	11001110	11001111	11010000	11010001	11010010	11010011	11010100	11010101	11010110	11010111	11011000	11011001	11011010	11011011	11011100	11011101	11011110	11011111	11100000	11100001	11100010	11100011	11100100	11100101	11100110	11100111	11101000	11101001	11101010	11101011	11101100	11101101	11101110	11101111	11110000	11110001	11110010	11110011	11110100	11110101	11110110	11110111	11111000	11111001	11111010	11111011	11111100	11111101	11111110	11111111

0	1	2	3	4	5	6	7	8	9	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z				
00		-	u0000000		-	u0000000		-	u0000000		-	u0000000		-	u0000000		-	u0000000		-	u0000000		-	u0000000		-	u0000000		-	u0000000		-	u0000000		-	u0000000			
01	-	u	0000000		-	u	0000000		-	u	0000000		-	u	0000000		-	u	0000000		-	u	0000000		-	u	0000000		-	u	0000000		-	u	0000000		-	u	0000000
02		1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000
03		1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000
04		1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000
05		1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000
06		1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000
07		1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000
08		1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000
09		1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000
0A		1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000
0B		1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000			1	0000000
0C		1	0000000			1	0000000			1	0000000																												

MATHEMATICAL RESEARCH BRANCH
 PROGRAM NAME: LS
 NUMBER OF COMPONENTS IS: 0
 NUMBER OF DATA POINTS IS: 7

C	I	OC	k
1	.101000+01	-.000000	.100000+01
1	.102000+01	-.000000	.100000+01
1	.103000+01	-.000000	.100000+01
1	.201000+01	-.000000	.100000+01
1	.202000+01	-.000000	.100000+01
1	.203000+01	-.000000	.100000+01
1	.301000+01	-.000000	.100000+01

[illegible]

ADJUSTABLE		DEPENDENT		FIXED	VALUE
INITIAL	ESTIMATE	MIN	MAX		
				LAMBDA (0, 1) =	.9526500-00
				LAMBDA (1, 2) =	.1450000-01
				LAMBDA (1, 3) =	.3283000-01
				LAMBDA (2, 1) =	-.1900000+01
				LAMBDA (0, 2) =	.4000000-00
				LAMBDA (2, 3) =	.6000000-00
				LAMBDA (3, 1) =	.7700000-01
				LAMBDA (3, 2) =	.3000000-00
				LAMBDA (0, 3) =	.2700000-00

10. INDEPENDENT STATISTICAL CONSTRAINTS

***NO ADJUSTABLE LAMBDAS. ITERATIONS SET TO 4E6. **19*

Math111	1	2	3
row 1	.1295710+01	.0000000	.0000000
row 2	.0000000	.2133503-00	.0000000
row 3	.0000000	.0000000	.7327220-02

SOLUTION

X-11.02

MODEL CODE= 3
ESTIMATE OF SIG FROM READ-IN DATA= .0000000

PARAMETER VALUES

ADJUSTABLE PARAMETERS

DEPENDENT PARAMETERS

FIXED PARAMETERS

D	C	T	GC/R	K	GC	GO	GO-OC	GC/GO
1	1	.100000-01	.600997-01	.100000+01	.600997-01	.000000	-.600997-01	.0000
2	1	.200000-01	.247164-01	.100000+01	.247164-01	.000000	-.247164-01	.0000
3	1	.300000-01	-.455086-01	.100000+01	-.455086-01	.000000	.455086-01	.0000
4	1	.101000+01	.123772+01	.100000+01	.123772+01	-.000000	-.123772+01	.0000
5	1	.102000+01	.571117-01	.100000+01	.571117-01	-.000000	-.571117-01	.0000
6	1	.103000+01	.266370-01	.100000+01	.266370-01	-.000000	-.266370-01	.0000
7	1	.201000+01	.120600+01	.100000+01	.120600+01	-.000000	-.120600+01	.0000
8	1	.202000+01	.135467-00	.100000+01	.135467-00	-.000000	-.135467-00	.0000
9	1	.203000+01	.162134-00	.100000+01	.162134-00	-.000000	-.162134-00	.0000
10	1	.301000+01	-.263804-01	.100000+01	-.263804-01	-.000000	.263804-01	.0000
11	1	.302000+01	.536388-01	.100000+01	.536388-01	.000000	-.536388-01	.0000
12	1	.303000+01	.143204-00	.100000+01	.143204-00	.000000	-.143204-00	.0000

SUM SQUARES AFTER 0 ITERATIONS IS .30357891+01

COMP 1= .3035769+01

SIG AFTER 0 ITERATIONS IS .43368416-00

***NO ADJUSTABLE PARAMETERS**b7*

SOLUTION TIME= .00000

. SAARZ3 MAT003.01 SIMULATL SIMILARITY TRANSFORMATION, OPTION B

RUNNING TIME= .00000

Lotka Oscillator - Simulate

Solve: $\frac{df_1}{dt} = 0$

$$f_1(0) = 1$$

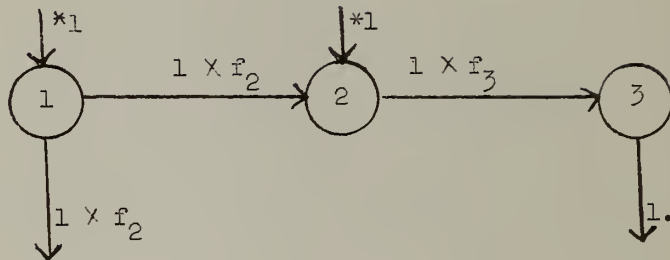
$$\frac{df_2}{dt} = f_2 - f_2 f_3$$

$$f_2(0) = 1$$

$$\frac{df_3}{dt} = f_2 f_3 - f_3$$

$$f_3(0) = 0$$

Schematic:



1	2	3	4	5	6	7	8
1234567890123456789012345678901234567890123456789012345678901234567890							

2	saan23	nan004.01	lotka oscillator	simulation example			1
2.		3					2
4			.01	.98		.98	3
2.							4
200.		.1		100.			
3.							
200.		.1		100.			
20							0
1		1.					
2		1.					
3		1.					
20							1
20							2
2	1	1.				2	
0	1	-1.				2	
3	2	1.				3	
0	3	1.					
20							3
20							4
20							5
20							0

1	2	3	4	5	6	7	8
1234567890123456789012345678901234567890123456789012345678901234567890							

SECTION XI

REFERENCES

Theory

- M. Berman and R. Schoenfeld. Invariants in experimental data on linear kinetics and the formulation of models. J. Appl. Phys. 27: 1361-1370, Nov. 1956.
- M. Berman and R. Schoenfeld. Information Content of Tracer Data with Respect to Steady State Systems. Symposium on Information Theory in Biology, H. P. Yockey, ed., Pergamon Press, pgs. 181-6, 1958.
- M. Berman, E. Shahn and M. F. Weiss. The routine fitting of kinetic data to models: A mathematical formalism for digital computers. Biophys. J., 2: 275, 1962.
- M. Berman, M. F. Weiss and E. Shahn. Some formal approaches to the analysis of kinetic data in terms of linear compartmental systems. Biophys. J., 1962, 2, 289.
- M. Berman. A postulate to aid in model building. J. Theoret. Biol. 4, 229-236, 1963.
- M. Berman. The formulation and testing of models. Ann. N. Y. Acad. Sci., 108: 182-194, 1963.
- M. Berman. Incomplete data and models. Proc. 6th IBM Computer Symposium, 1964.
- M. Berman. Compartmental analysis in kinetics. Computers in Biomedical Research, vol. 2, Chapter VII+ (Eds. R. Stacy and B. Waxman). Academic Press, N. Y., 1965.
7. L. Collatz. The Numerical Treatment of Differential Equations
Third edition. Springer-Verlag, 1960
8. T. W. Anderson. An Introduction to Multivariate Statistical Analysis.
John Wiley and Sons, Inc. New York, 1958.

Applications

- C. G. Lewallen, M. Berman and J. E. Rall. Studies of Iodoalbumin metabolism. I. A mathematical approach to the kinetics. J. Clin. Invest. 38: 66-87, Jan. 1959.
- S. Segal, M. Berman and A. Blair. The metabolism of variously C¹⁴ labeled glucose in man and an estimation of the extent of glucose metabolism by the hexose monophosphate pathway. J. Clin. Invest. 40: 1263-79, July 1961.
- M. Berman. Application of Differential equations to the study of the thyroid system. Proc. Berkeley Symposium on Math. Stat. and Prob., 1960. Univ. of Calif. Press, 1961.
- C. Ayers, J. O. Davis, F. Lieberman, C. C. J. Carpenter and M. Berman. The effect of chronic hepatic venous congestion on the metabolism of D, L-Aldosterone and D-Aldosterone. J. Clin. Invest., 41: 884, 1962.
- L. E. Rosenberg, M. Berman and S. Segal. Studies of the kinetics of amino acid transport, incorporation into protein and oxidation in kidney-cortex slices. Biochim. Biophys. Acta, 71: 664-675, 1963.
- W. E. Mayberry, J. E. Rall, M. Berman and D. Bertoli. Kinetics of iodination, III. Iodination of N-acetyl-L-tyrosine and N-acetyl-3-iodo-L-tyrosine studies in pH stat. system. Biochem. 4: 1965-1972, 1965.
- L. V. Avioli and M. Berman. Mg²⁸ kinetics in man. J. Appl. Physiol. 21: 1688-94, Nov. 1966.

- M. Berman. The iodine pool. In P. Bergner, E. E. Lushbaugh and C. C. Lushbaugh (Eds.): Compartments, Pools and Space in Medical Physiology. Oak Ridge, Tennessee, AEC Symposium Series CONF 661010. In press (1967).
- G. L. Turco, F. Ghemi, G. Molino and G. Segre. The kinetics of I^{131} rose bengal in normal and cirrhotic subjects studied by compartmental analysis and a digital computer. J. of Lab. and Clin. Med. 67: 983-993, June 1966.
- H. Hoch, S. L. Sinnett, P. O. Miller and I. B. Mahady. Dialyzable thyroid hormone-binding material in human serum. Biochemistry 4: 931-939, May 1965.
- A. H. Tashjian, and G. D. Whedon. Kinetics of human citrate metabolism: studies in normal subjects and in patients with bone disease. J. of Clin. Endocrin. and Metab. 23: 1029-1043, Oct. 1963.
- M. B. Burg, E. F. Grollman and J. Orloff. Sodium and potassium flux of separated renal tubules. Am. J. of Physiology 206: 483-491, March 1964.
- R. B. Marimont. Numerical studies of the Fuortes-Hodgkin limulus model. J. Physiol. 179: 489-497, 1965.
- W. Rall. Theoretical significance of dendritic trees for neuronal input-output relations. In Neural Theory and Modeling. R. F. Reiss, editor, Stanford University Press, 1964.
- G. L. Turco, P. De Filippi and G. Segre. The kinetics of intestinal absorption of radio-hippuran in control subjects and in patients with intestinal malabsorption. J. Nuclear Med. and Biol. 1966.

G. D. Thorburn, H. H. Kopald, J. A. Herd, M. Hollenberg, C. C. C.

O'Morchoe and A. C. Barger. Intrarenal distribution of nutrient blood flow determined with Krypton⁸⁵ in the unanesthetized dog.

Circulation Research Vol. XIII, No. 4, Oct. 1963.

S. H. Cohn, S. R. Bozzo, J. E. Jesseph, C. Constantinides, D. R. Huene and

E. A. Gusmano. Formulation and testing of a compartmental model for calcium metabolism in man. Brookhaven National Laboratory Report 8693.

S. H. Cohn, S. Bozzo, N. Glatstein, C. Constantinides, J. Litvak and

E. A. Gusmano. Formulations of a compartmental model in a study of partial parathyroid deficiency. Metabolism, 13: 1356-1368, Nov. 1964.

SECTION XII

APPENDIX

THE UNIVERSITY OF IOWA

IOWA CITY, IOWA 52240



December 22, 1966

College of Engineering
Department of Chemical Engineering
Area 319: 353-4875

Dr. Mones Berman
National Institute of Arthritis
and Metabolic Diseases
Bethesda 14, Maryland

Dear Dr. Berman:

Here is a description of the way we
have adapted your SAAM 22 program to our 7044
computer. You asked for this in our telephone
conversation of a few days ago.

Sincerely,

James O Osburn
James O. Osburn, Professor
Dept. of Chemical Engineering

w

Computer Center
University of Iowa
Iowa City, Iowa

SAAM 22 has been up-dated to Fortran IV language with one MAP subroutine for use on a 7044 system. The number of data points was reduced to 100 and all items dimensioned at 61 were reduced to 50. DS and CAT were eliminated. These changes were necessary in order to have the program fit the computer. Link 4 is the largest link and leaves approximately 1090 decimal of unused core.

At the University of Iowa we use an object deck tape to up-date the programs, and when also used for execution, load time is about 7 minutes. We have also made a reload tape which reduces load time to almost zero. The University of Iowa will copy these tapes if tapes are furnished. To up-date the object deck tape the Delete card is used.

The sustem including 1Ø CS uses 8 files - FT000, FT001, S.FBØU, S.FBPP, S.FBIN, FT003, FT004 and FT001. The following subroutines are also on the system:

CHNRTN	FO4
CNSTNT	FO5
PØSTX	FO6
IØS	FO7
RWD	FPR
ICV	RWB
INTJ	ACV
RWT	ECV
UTV	HCV
FPT	XCV
XEM	FFC
XIT	INVERT*
FOO	This is a U. of I. sub-
FO1	routine and can be furnished.
FO2	
FO3	

The Main Line contains SR43 and SCH.

The 43 is a NIH number and SCH is a U. of I. subroutine.

CLKRD is a MAP subroutine from U. of I.

The rest of the links are arranged as described in SAAM 22 literature and the subroutine numbers and names are kept the same. With the reload tape the following control cards are used:

```
$ IBSYS
$ JOB
$ COMMENT USE RELOAD TAPE 283
$ *READY SCRATCH TAPES ON B-S AND B-6.
$ PAUSE MOUNT TAPE 283 ON B4
$ TIME      15
$ PAGE      300
$ IBJOB NIH
$ RELOAD U09
```

5	10	15	20	25	30	35	40	45	50
-5	6	7	3	2	1	4	8	8	8

These are tape assignments.

NTAPE0 = 5, NTAPE1 = 6, etc.

Data Decks as used for SAAM 22, 9B20, etc.

	9	16	
7	9	SAAM	FINAL CARDS

```
$ IBSYS
$ CLOSE          S.SU09,REMOVE
```

For the object Deck Tapes the following controls have been used.

```
$ IBSYS
$ JØB
$ TIME
$ COMMENT
$ PAUSE MØUNT TAPE PYB20 AS INPUT ØN UOS
$ EXECUTE      UPDATE
$ RUN UPDATE
$ ØBTAIN PRINT  SUMMARY
$ NUMBER ZOOOOOOO
$ DELETE
$ IB JOB NIH MAP, NØ SØURCE
$ CHAIN      SAAM 22
```

```
$ FILE      'FTCOO.', UOO, UOO, BLØCK=15,SINGLE, REEL ,
              SCRTCH, TYPE3
$ ETC        LRL=14, RCT=1, EØR= REØRX., EØF=REOFX.
              ERR=RERRX.
$ FILE      'FTCO1., UO5, UO5, BLØCK=15, SINGLE,
              REEL, SCRTCH, TYPE3

$ ETC        LRL=14, .....
$ FILE      'S.FBØU', ØU, ØU, BLØCK=100, MIXED, TYPE3
$ FILE      'S.FBPP', PP, PP, BLØCK=100, MIXED,SINGLE
              TYPE3, LRL=14
$ FILE      'S.FBIN', IN, IN, BLOCK=150, SINGLE,
              MIXED, TYPE3
$ FILE      'FTCO3', UO6, UO6, BLØCK=15, SINGLE,
              REEL, SCRTCH, TYPE3
$ ETC        LRL=14, . . . . .
$ FILE      'FTCO4', UO7, UO7, BLØCK=15, . . . . .
$ ETC        LRL=14, . . . . .
```

OBJECT DECKS

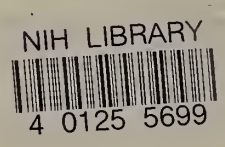
```
$ ENTRY      SR89
$ ENDCH
    5        6        7        3        2        1        4        8        8        8
```

DATA DECKS

```
          9          16
7    9    SAAM      FINAL CARDS
```

```
$ IBSYS
$ CLØSE S.SUO6
$ IBSYS
$ SWITCH S.S.IN1, S.SUO6
$ STOP
$ STOP
```

For a listing, write Mike Hensel, University Computer Center, Iowa City. Probably 3 tapes would be required.





<http://nihlibrary.nih.gov>

10 Center Drive
Bethesda, MD 20892-1150
301-496-1080

NIH LIBRARY



3 1496 00268 7419

~~FEB 20 1989~~

~~DEC 04 1990~~

FEB 00 1991

~~FEB 06 1991~~

~~APR 15 1991~~

~~MAY 03 1991~~

~~APR 15 1991~~

~~FEB 15 1991~~